



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:51 PM UTC

PDB ID : 5X3X / pdb_00005x3x
Title : 2.8Å resolution structure of a cobalt energy-coupling factor transporter-CbiMQO
Authors : Bao, Z.; Qi, X.; Wang, J.; Zhang, P.
Deposited on : 2017-02-09
Resolution : 2.79 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

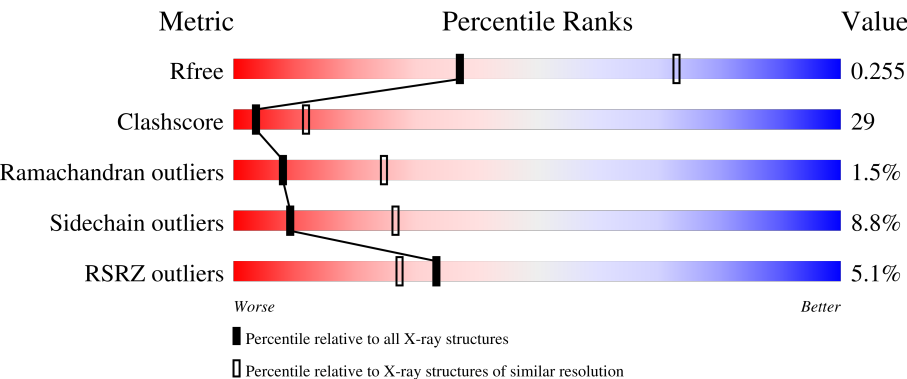
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	280	3% 62% 31% 6% .
1	B	280	2% 68% 27% . .
1	a	280	9% 61% 30% 6% .
1	b	280	7% 66% 26% 5% .
2	M	222	3% 59% 24% 9% . 7%

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Mol	Chain	Length	Quality of chain
2	m	222	4% 53% 30% 9% 8%
3	Q	244	7% 57% 32% 7% •
3	q	244	7% 58% 29% 11% ••

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14966 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cobalt ABC transporter ATP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	280	Total	C	N	O	S	0	0	0
			2067	1300	380	382	5			
1	B	280	Total	C	N	O	S	0	0	0
			2069	1301	380	383	5			
1	a	279	Total	C	N	O	S	0	0	0
			2058	1295	376	382	5			
1	b	280	Total	C	N	O	S	0	0	0
			2069	1301	380	383	5			

- Molecule 2 is a protein called Cobalt transport protein CbiM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	207	Total	C	N	O	S	0	0	0
			1474	978	237	252	7			
2	m	205	Total	C	N	O	S	0	0	0
			1461	970	234	250	7			

- Molecule 3 is a protein called Uncharacterized protein CbiQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Q	243	Total	C	N	O	S	0	0	0
			1815	1175	333	301	6			
3	q	242	Total	C	N	O	S	0	0	0
			1807	1169	332	300	6			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	24	Total	O	0	0
			24	24		
4	B	19	Total	O	0	0
			19	19		

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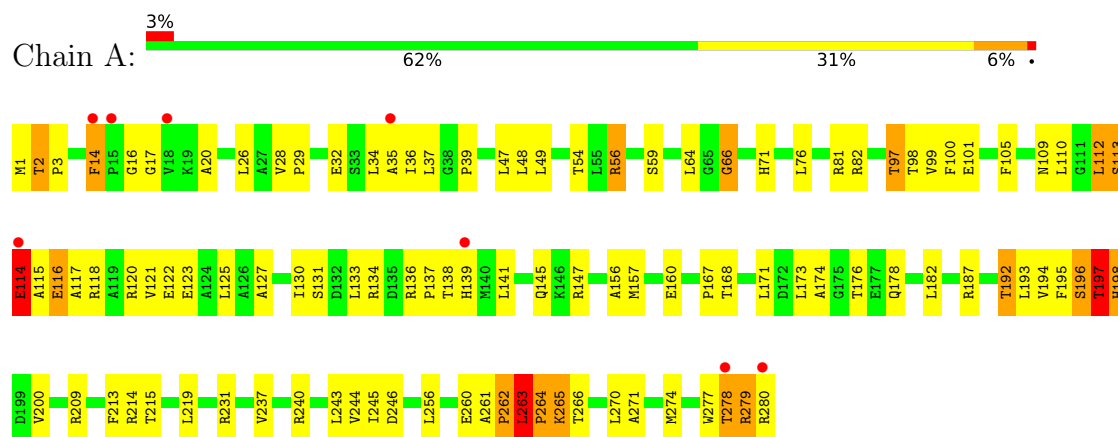
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	M	9	Total 9	O 9	0	0
4	Q	28	Total 28	O 28	0	0
4	a	19	Total 19	O 19	0	0
4	b	16	Total 16	O 16	0	0
4	m	13	Total 13	O 13	0	0
4	q	18	Total 18	O 18	0	0

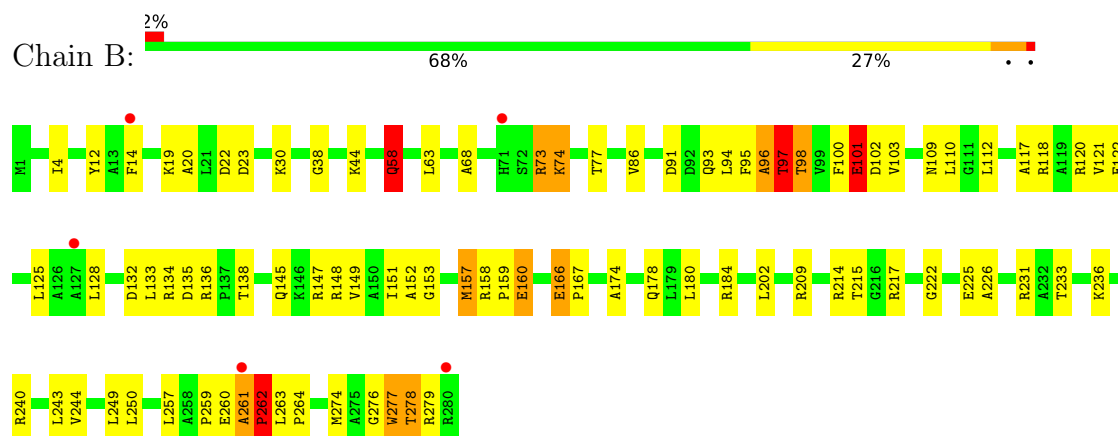
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

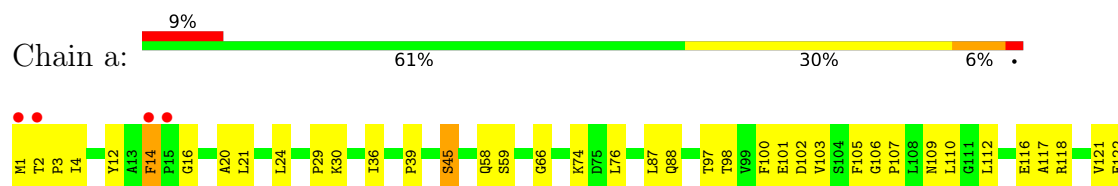
- Molecule 1: Cobalt ABC transporter ATP-binding protein

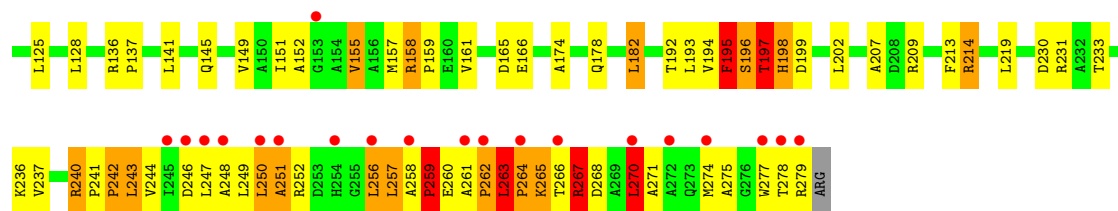


- Molecule 1: Cobalt ABC transporter ATP-binding protein

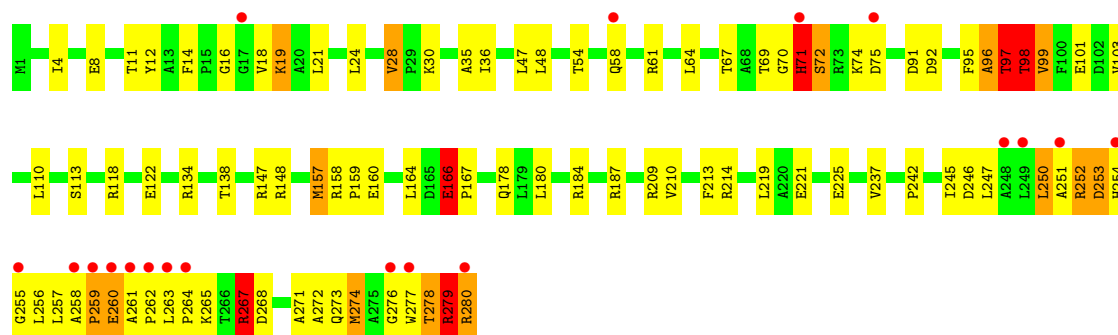


- Molecule 1: Cobalt ABC transporter ATP-binding protein

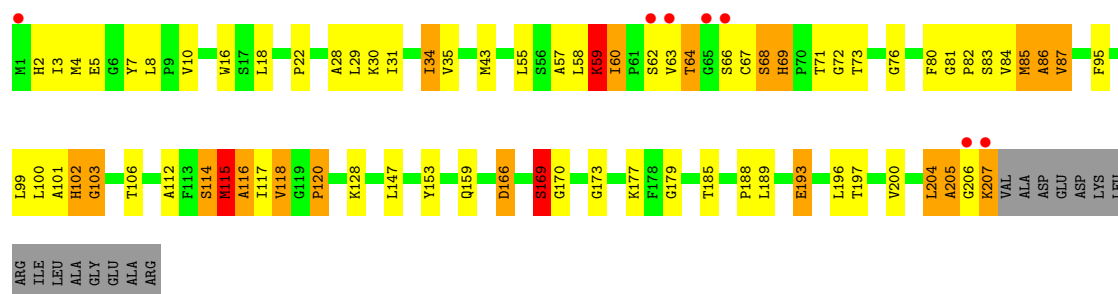




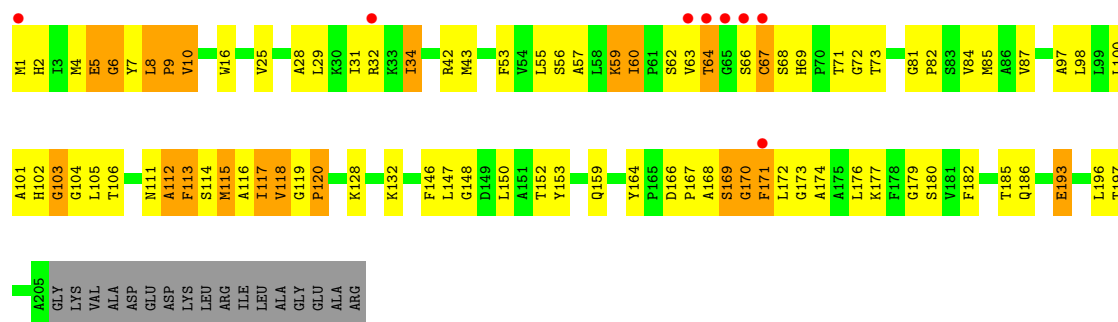
• Molecule 1: Cobalt ABC transporter ATP-binding protein



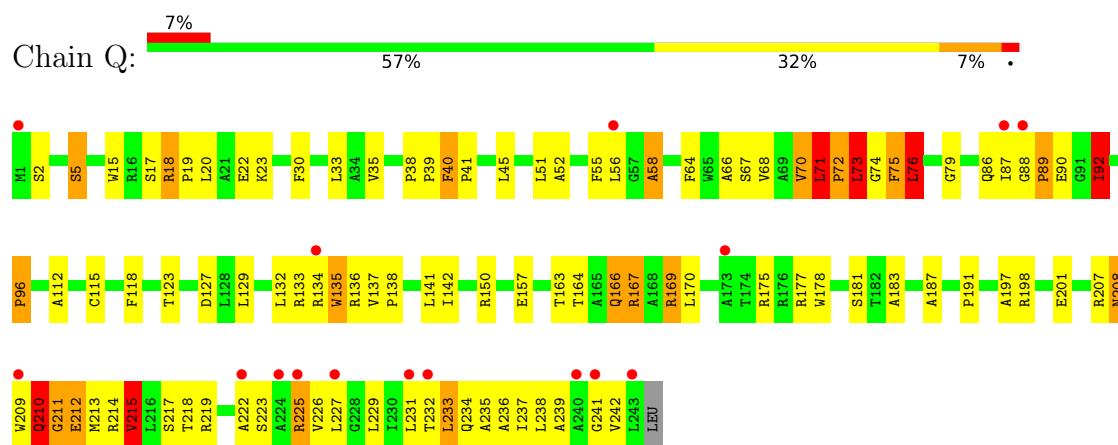
• Molecule 2: Cobalt transport protein CbiM



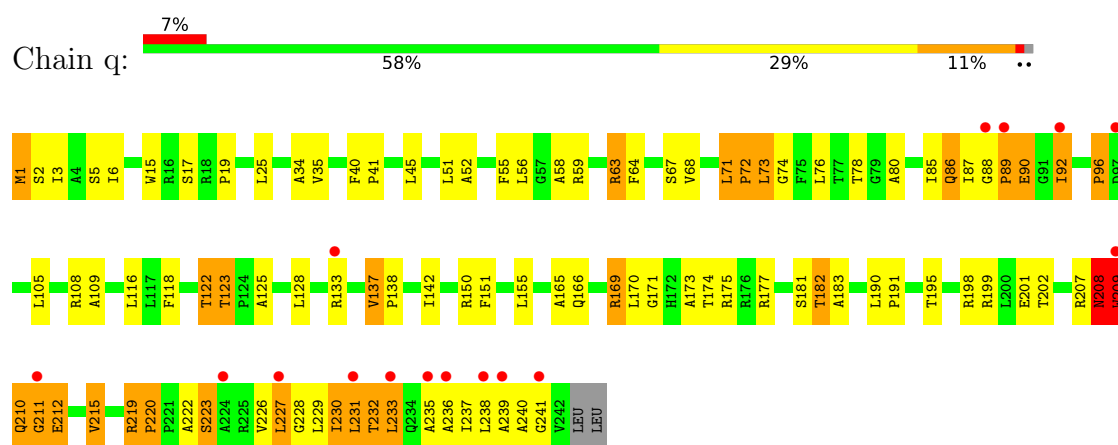
• Molecule 2: Cobalt transport protein CbiM



• Molecule 3: Uncharacterized protein CbiQ



• Molecule 3: Uncharacterized protein CbiQ



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	63.68Å 220.56Å 301.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.33 – 2.79 48.33 – 2.79	Depositor EDS
% Data completeness (in resolution range)	87.0 (48.33-2.79) 87.0 (48.33-2.79)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.47 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.214 , 0.249 0.226 , 0.255	Depositor DCC
R_{free} test set	2376 reflections (4.43%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.071	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	14966	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2942e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.03	9/2096 (0.4%)	1.18	19/2847 (0.7%)
1	B	0.94	7/2098 (0.3%)	1.13	10/2850 (0.4%)
1	a	0.90	6/2087 (0.3%)	1.22	18/2836 (0.6%)
1	b	0.95	7/2098 (0.3%)	1.18	18/2850 (0.6%)
2	M	1.21	7/1508 (0.5%)	1.33	16/2059 (0.8%)
2	m	1.23	6/1495 (0.4%)	1.32	18/2043 (0.9%)
3	Q	1.02	5/1850 (0.3%)	1.30	20/2525 (0.8%)
3	q	1.03	2/1842 (0.1%)	1.36	23/2514 (0.9%)
All	All	1.03	49/15074 (0.3%)	1.25	142/20524 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2
1	b	0	1
3	Q	0	1
3	q	0	1
All	All	0	5

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	166	GLU	C-O	-12.70	1.18	1.23
1	A	198	HIS	C-O	-9.16	1.12	1.24
1	A	197	THR	C-O	-9.02	1.14	1.23
1	B	166	GLU	C-O	-8.71	1.19	1.23
1	B	96	ALA	CA-C	-8.03	1.46	1.53
3	q	209	TRP	CA-C	-7.82	1.43	1.52
1	a	196	SER	CA-C	7.75	1.61	1.52
1	A	194	VAL	C-O	-7.33	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	96	ALA	CA-C	-7.06	1.46	1.53
1	b	96	ALA	C-O	-6.96	1.17	1.24
1	a	193	LEU	C-O	-6.76	1.16	1.23
1	a	198	HIS	CG-ND1	-6.60	1.30	1.38
2	m	4	MET	C-O	-6.44	1.17	1.23
1	A	192	THR	CA-C	-6.40	1.45	1.52
1	a	194	VAL	C-O	-6.39	1.17	1.24
1	B	166	GLU	CA-C	-6.32	1.49	1.53
2	M	85	MET	C-O	-6.24	1.16	1.24
1	b	166	GLU	CA-C	-6.21	1.49	1.53
2	M	102	HIS	CG-ND1	-6.15	1.31	1.38
1	A	198	HIS	CG-ND1	-6.13	1.31	1.38
2	M	59	LYS	C-O	-6.04	1.16	1.24
2	m	112	ALA	C-O	-6.01	1.17	1.24
3	Q	215	VAL	C-O	-6.00	1.18	1.24
1	a	198	HIS	CD2-NE2	-5.86	1.31	1.37
1	B	96	ALA	C-O	-5.86	1.18	1.24
2	M	116	ALA	N-CA	-5.82	1.39	1.46
1	A	193	LEU	C-O	-5.72	1.16	1.24
2	m	87	VAL	C-O	-5.62	1.17	1.24
2	M	87	VAL	C-O	-5.61	1.17	1.24
1	B	98	THR	C-O	-5.59	1.17	1.23
1	b	259	PRO	N-CD	5.54	1.55	1.47
1	b	71	HIS	CG-ND1	-5.51	1.32	1.38
1	A	196	SER	C-O	-5.47	1.17	1.23
1	b	98	THR	C-O	-5.46	1.17	1.23
3	Q	129	LEU	C-O	-5.45	1.17	1.24
2	M	69	HIS	CA-C	-5.40	1.47	1.52
1	B	101	GLU	C-O	-5.38	1.17	1.24
3	Q	70	VAL	CA-C	5.34	1.59	1.52
2	M	69	HIS	CG-ND1	-5.33	1.32	1.38
2	m	69	HIS	CA-C	-5.28	1.47	1.52
3	Q	169	ARG	C-O	-5.27	1.17	1.24
1	B	94	LEU	C-O	-5.24	1.17	1.24
2	m	69	HIS	CG-ND1	-5.23	1.32	1.38
1	A	192	THR	C-O	-5.22	1.17	1.24
3	Q	167	ARG	C-O	-5.20	1.18	1.24
2	m	120	PRO	C-O	-5.05	1.18	1.24
1	A	277	TRP	NE1-CE2	-5.00	1.31	1.37
1	a	240	ARG	C-O	-5.00	1.19	1.24
3	q	125	ALA	C-O	-5.00	1.17	1.24

All (142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	70	VAL	N-CA-C	18.43	129.34	110.72
3	q	211	GLY	N-CA-C	13.99	129.41	112.49
1	B	277	TRP	N-CA-C	13.00	125.53	111.36
2	M	87	VAL	N-CA-C	11.03	121.86	110.72
1	a	197	THR	N-CA-C	-10.83	92.45	109.23
1	b	96	ALA	N-CA-C	10.62	124.45	108.31
1	a	66	GLY	N-CA-C	-10.53	100.42	115.27
2	m	6	GLY	N-CA-C	-10.49	98.08	112.13
2	m	82	PRO	N-CA-C	10.37	127.94	113.53
3	q	40	PHE	CA-C-N	-10.35	107.57	118.85
3	q	40	PHE	C-N-CA	-10.35	107.57	118.85
2	m	87	VAL	N-CA-C	10.22	121.04	110.72
1	a	198	HIS	N-CA-C	-10.16	87.61	107.62
2	m	81	GLY	CA-C-N	10.00	130.15	119.05
2	m	81	GLY	C-N-CA	10.00	130.15	119.05
2	M	118	VAL	N-CA-C	-9.85	98.47	112.35
1	a	198	HIS	CA-C-N	9.80	136.29	121.40
1	a	198	HIS	C-N-CA	9.80	136.29	121.40
2	m	5	GLU	N-CA-C	9.76	121.92	111.28
1	A	278	THR	N-CA-C	9.69	127.17	112.54
1	a	242	PRO	N-CA-C	-9.60	95.95	111.21
2	M	81	GLY	CA-C-N	9.40	129.48	119.05
2	M	81	GLY	C-N-CA	9.40	129.48	119.05
2	M	82	PRO	N-CA-C	9.39	126.58	113.53
3	Q	40	PHE	CA-C-N	-9.29	108.73	118.85
3	Q	40	PHE	C-N-CA	-9.29	108.73	118.85
1	a	267	ARG	N-CA-C	-9.22	101.13	112.38
1	a	259	PRO	CB-CA-C	-9.17	103.05	111.40
1	B	157	MET	N-CA-C	-8.95	97.24	110.48
1	b	157	MET	N-CA-C	-8.74	96.40	110.20
1	A	113	SER	N-CA-C	8.73	120.88	111.36
2	M	115	MET	CA-C-N	-8.71	109.16	120.65
2	M	115	MET	C-N-CA	-8.71	109.16	120.65
3	q	71	LEU	CA-C-N	-8.39	110.77	119.83
3	q	71	LEU	C-N-CA	-8.39	110.77	119.83
3	Q	233	LEU	N-CA-C	-8.37	102.33	112.54
1	A	66	GLY	N-CA-C	-8.32	104.10	114.92
1	B	278	THR	CB-CA-C	-8.15	105.13	115.89
3	q	212	GLU	N-CA-C	-8.04	96.58	109.76
3	q	173	ALA	N-CA-C	7.96	119.74	111.14
1	A	56	ARG	CA-C-N	-7.94	112.66	120.52
1	A	56	ARG	C-N-CA	-7.94	112.66	120.52
3	q	219	ARG	CA-C-N	7.87	125.33	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	q	219	ARG	C-N-CA	7.87	125.33	119.66
1	b	96	ALA	CB-CA-C	-7.74	107.64	116.54
3	q	209	TRP	CA-C-N	7.66	130.54	120.28
3	q	209	TRP	C-N-CA	7.66	130.54	120.28
2	M	114	SER	CA-C-N	-7.58	110.59	120.44
2	M	114	SER	C-N-CA	-7.58	110.59	120.44
2	M	116	ALA	CA-C-N	-7.57	110.87	120.56
2	M	116	ALA	C-N-CA	-7.57	110.87	120.56
1	b	158	ARG	CA-C-N	-7.36	112.74	120.03
1	b	158	ARG	C-N-CA	-7.36	112.74	120.03
3	Q	73	LEU	CA-C-N	-7.19	111.96	119.94
3	Q	73	LEU	C-N-CA	-7.19	111.96	119.94
3	Q	76	LEU	N-CA-C	7.03	118.94	111.28
1	a	158	ARG	CA-C-N	6.95	127.40	120.52
1	a	158	ARG	C-N-CA	6.95	127.40	120.52
3	Q	71	LEU	CA-C-O	6.91	124.69	117.98
1	b	267	ARG	N-CA-C	6.84	118.53	111.14
3	q	210	GLN	N-CA-CB	-6.84	100.07	110.12
3	q	220	PRO	O-C-N	6.70	124.30	121.15
1	a	270	LEU	N-CA-C	-6.70	103.98	111.28
3	q	169	ARG	N-CA-C	-6.58	101.85	110.53
1	b	71	HIS	N-CA-C	6.43	120.73	113.01
1	A	193	LEU	N-CA-C	-6.43	98.92	109.40
1	a	195	PHE	N-CA-C	-6.40	99.77	109.95
1	a	256	LEU	N-CA-C	-6.39	104.36	111.71
1	b	258	ALA	N-CA-C	6.38	118.92	110.36
2	m	118	VAL	CA-C-N	-6.30	111.98	121.87
2	m	118	VAL	C-N-CA	-6.30	111.98	121.87
3	q	209	TRP	N-CA-CB	6.29	119.68	109.69
3	Q	135	TRP	N-CA-C	-6.27	101.70	110.35
1	b	96	ALA	CA-C-N	6.22	133.42	121.54
1	b	96	ALA	C-N-CA	6.22	133.42	121.54
2	m	98	LEU	N-CA-C	6.16	118.08	111.36
1	B	96	ALA	N-CA-C	6.14	117.64	108.31
3	Q	211	GLY	N-CA-C	6.11	119.85	111.54
1	B	96	ALA	CB-CA-C	-6.11	109.52	116.54
1	B	261	ALA	N-CA-C	6.09	115.96	108.11
2	M	59	LYS	CA-C-N	-6.05	118.06	123.33
2	M	59	LYS	C-N-CA	-6.05	118.06	123.33
1	a	275	ALA	N-CA-C	-6.02	105.93	113.28
2	M	169	SER	N-CA-C	5.95	121.45	113.72
3	Q	132	LEU	CA-C-N	5.91	128.20	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	132	LEU	C-N-CA	5.91	128.20	120.28
1	A	14	PHE	CA-C-N	-5.88	112.50	119.84
1	A	14	PHE	C-N-CA	-5.88	112.50	119.84
3	q	137	VAL	CA-C-N	5.85	125.81	119.78
3	q	137	VAL	C-N-CA	5.85	125.81	119.78
3	Q	219	ARG	CA-C-N	5.84	126.40	120.38
3	Q	219	ARG	C-N-CA	5.84	126.40	120.38
1	b	28	VAL	N-CA-C	5.83	113.84	107.60
1	A	265	LYS	N-CA-CB	-5.82	107.53	114.17
1	b	274	MET	N-CA-C	-5.80	105.30	112.38
3	Q	92	ILE	N-CA-C	5.78	115.93	107.37
1	a	263	LEU	N-CA-C	5.78	122.59	109.81
3	q	210	GLN	CA-C-N	5.78	126.24	119.94
3	q	210	GLN	C-N-CA	5.78	126.24	119.94
1	b	99	VAL	CB-CA-C	-5.77	104.35	112.14
3	Q	72	PRO	N-CA-C	-5.70	105.61	113.53
2	m	67	CYS	CA-C-N	-5.68	115.16	123.00
2	m	67	CYS	C-N-CA	-5.68	115.16	123.00
1	A	278	THR	CA-C-N	-5.65	115.21	123.00
1	A	278	THR	C-N-CA	-5.65	115.21	123.00
2	m	170	GLY	N-CA-C	-5.64	105.04	112.82
1	A	20	ALA	N-CA-C	-5.61	104.79	111.69
2	m	113	PHE	CA-C-N	-5.58	113.03	120.63
2	m	113	PHE	C-N-CA	-5.58	113.03	120.63
1	a	45	SER	N-CA-C	5.42	117.26	111.36
1	B	160	GLU	N-CA-C	-5.38	105.86	112.90
3	q	171	GLY	N-CA-C	5.38	120.87	113.99
1	A	264	PRO	CA-C-N	-5.35	116.97	126.45
1	A	264	PRO	C-N-CA	-5.35	116.97	126.45
2	M	205	ALA	N-CA-C	-5.34	105.54	111.36
1	A	198	HIS	O-C-N	-5.33	116.42	122.23
1	b	99	VAL	N-CA-C	5.33	116.06	110.62
1	A	2	THR	CA-C-N	-5.33	114.43	119.76
1	A	2	THR	C-N-CA	-5.33	114.43	119.76
1	a	14	PHE	CA-C-N	-5.32	113.19	119.84
1	a	14	PHE	C-N-CA	-5.32	113.19	119.84
3	q	230	ILE	N-CA-C	-5.30	105.22	110.62
2	m	112	ALA	CA-C-N	-5.27	113.59	120.44
2	m	112	ALA	C-N-CA	-5.27	113.59	120.44
2	m	111	ASN	N-CA-C	5.25	117.00	111.28
2	M	86	ALA	N-CA-C	-5.24	105.47	111.07
1	b	258	ALA	CA-C-N	-5.23	113.31	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	258	ALA	C-N-CA	-5.23	113.31	119.84
3	Q	73	LEU	N-CA-C	-5.21	105.60	111.28
3	q	72	PRO	CA-C-O	-5.18	115.69	121.23
1	B	73	ARG	N-CA-C	-5.17	106.48	112.89
1	B	158	ARG	CA-C-N	-5.13	115.28	120.31
1	B	158	ARG	C-N-CA	-5.13	115.28	120.31
2	m	169	SER	N-CA-C	5.10	120.36	114.04
3	Q	58	ALA	CA-C-N	-5.03	116.29	123.03
3	Q	58	ALA	C-N-CA	-5.03	116.29	123.03
3	Q	22	GLU	N-CA-C	5.02	116.56	111.14
1	b	28	VAL	CA-C-N	5.02	124.78	119.76
1	b	28	VAL	C-N-CA	5.02	124.78	119.76
1	A	99	VAL	CB-CA-C	-5.02	105.37	112.14
1	A	28	VAL	N-CA-C	5.00	112.96	107.60
3	q	128	LEU	N-CA-C	5.00	116.81	111.36

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	58	GLN	Sidechain
1	B	95	PHE	Peptide
3	Q	208	ASN	Peptide
1	b	95	PHE	Peptide
3	q	208	ASN	Peptide

5.2 Too-close contacts [\(i\)](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2067	0	2150	131	0
1	B	2069	0	2158	97	0
1	a	2058	0	2145	161	0
1	b	2069	0	2158	126	0
2	M	1474	0	1552	102	0
2	m	1461	0	1536	116	0
3	Q	1815	0	1950	152	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	q	1807	0	1939	128	2
4	A	24	0	0	8	0
4	B	19	0	0	13	0
4	M	9	0	0	1	0
4	Q	28	0	0	25	0
4	a	19	0	0	5	0
4	b	16	0	0	4	0
4	m	13	0	0	1	0
4	q	18	0	0	27	0
All	All	14966	0	15588	883	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (883) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:207:LYS:CE	3:Q:191:PRO:HG3	1.48	1.40
3:Q:71:LEU:CD1	3:Q:72:PRO:HD3	1.57	1.33
1:a:278:THR:O	1:a:279:ARG:CG	1.76	1.32
1:A:98:THR:CG2	1:A:101:GLU:HB2	1.59	1.32
1:a:243:LEU:CD1	1:b:267:ARG:HD2	1.60	1.30
1:a:263:LEU:C	1:a:263:LEU:HD13	1.53	1.29
3:q:118:PHE:O	3:q:122:THR:HG23	1.34	1.26
3:q:233:LEU:HD23	3:q:233:LEU:O	1.33	1.25
3:Q:71:LEU:HD13	3:Q:72:PRO:HD3	1.22	1.21
3:Q:71:LEU:HD12	3:Q:72:PRO:CD	1.70	1.21
1:b:278:THR:CG2	1:b:279:ARG:H	1.54	1.20
3:Q:229:LEU:HD12	4:Q:303:HOH:O	1.37	1.20
1:a:277:TRP:CB	1:b:278:THR:HG21	1.71	1.20
3:Q:73:LEU:HD13	3:Q:73:LEU:C	1.61	1.19
1:b:96:ALA:O	1:b:97:THR:HG23	1.37	1.19
1:B:277:TRP:O	1:B:278:THR:HG22	1.44	1.17
3:Q:41:PRO:HD2	4:Q:301:HOH:O	1.45	1.16
3:q:118:PHE:O	3:q:122:THR:CG2	1.95	1.15
1:a:243:LEU:HD13	1:b:267:ARG:HD2	1.24	1.15
1:A:98:THR:HG23	1:A:101:GLU:HB2	1.17	1.14
1:A:263:LEU:HD12	1:A:263:LEU:C	1.69	1.14
3:Q:87:ILE:CD1	3:Q:92:ILE:HG22	1.77	1.14
1:a:277:TRP:HB3	1:b:278:THR:CG2	1.77	1.13
3:Q:87:ILE:CD1	3:Q:92:ILE:CG2	2.27	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:207:LYS:NZ	3:Q:191:PRO:HG3	1.64	1.12
3:q:25:LEU:HD23	3:q:230:ILE:HD11	1.31	1.11
1:a:244:VAL:HG13	1:a:270:LEU:CD1	1.80	1.11
1:a:252:ARG:HB2	1:a:257:LEU:CD2	1.81	1.11
1:A:279:ARG:NH2	1:A:279:ARG:HG3	1.48	1.09
3:Q:40:PHE:N	4:Q:301:HOH:O	1.84	1.09
3:q:233:LEU:HD23	3:q:233:LEU:C	1.76	1.09
1:A:279:ARG:HH21	1:A:279:ARG:CG	1.64	1.08
1:a:243:LEU:HD13	1:b:267:ARG:CD	1.83	1.08
3:Q:135:TRP:HB3	4:Q:304:HOH:O	1.52	1.08
1:b:70:GLY:O	1:b:75:ASP:HB3	1.55	1.07
1:b:278:THR:HG23	1:b:279:ARG:N	1.67	1.07
2:m:59:LYS:H	2:m:59:LYS:HD2	1.20	1.07
3:Q:73:LEU:HD13	3:Q:73:LEU:O	1.54	1.07
1:B:98:THR:OG1	1:B:101:GLU:HG3	1.53	1.07
2:M:116:ALA:O	2:M:120:PRO:HD2	1.54	1.06
1:a:278:THR:O	1:a:279:ARG:HG2	0.89	1.06
2:m:168:ALA:HB3	3:q:87:ILE:O	1.52	1.06
3:q:58:ALA:HB1	4:q:305:HOH:O	1.53	1.06
2:M:207:LYS:HE2	3:Q:191:PRO:CG	1.85	1.05
3:Q:71:LEU:HD12	3:Q:71:LEU:H	1.16	1.05
3:Q:87:ILE:HD13	3:Q:92:ILE:CG2	1.86	1.05
1:A:98:THR:CG2	1:A:101:GLU:CB	2.34	1.05
2:m:59:LYS:O	2:m:60:ILE:HD13	1.55	1.05
3:Q:87:ILE:HD13	3:Q:92:ILE:HG22	1.32	1.04
1:b:277:TRP:HA	1:b:278:THR:HB	1.36	1.04
2:M:177:LYS:HE2	3:Q:87:ILE:CG1	1.85	1.04
1:b:278:THR:HG23	1:b:279:ARG:H	0.89	1.04
3:q:226:VAL:HG23	4:q:304:HOH:O	1.58	1.04
3:Q:68:VAL:O	3:Q:71:LEU:HD11	1.58	1.03
3:Q:71:LEU:HD12	3:Q:72:PRO:HD2	1.39	1.03
2:M:177:LYS:HE2	3:Q:87:ILE:HG12	1.38	1.03
3:Q:71:LEU:HD12	3:Q:71:LEU:N	1.66	1.03
3:Q:73:LEU:C	3:Q:73:LEU:CD1	2.30	1.03
2:m:167:PRO:HB2	3:q:86:GLN:NE2	1.74	1.03
1:a:278:THR:C	1:a:279:ARG:HG2	1.83	1.02
3:Q:71:LEU:CD1	3:Q:71:LEU:H	1.60	1.02
1:a:243:LEU:HD12	1:b:267:ARG:HD2	1.38	1.02
1:B:261:ALA:HB1	1:B:262:PRO:HD2	1.40	1.02
1:B:278:THR:HG23	1:B:279:ARG:N	1.71	1.02
1:a:263:LEU:HD13	1:a:264:PRO:N	1.73	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:71:LEU:CD1	3:Q:72:PRO:CD	2.30	1.01
1:a:265:LYS:HD2	1:a:265:LYS:O	1.61	1.01
3:q:226:VAL:N	4:q:304:HOH:O	1.94	1.00
1:A:98:THR:HG22	1:A:101:GLU:OE1	1.60	0.99
1:A:263:LEU:C	1:A:263:LEU:CD1	2.33	0.99
2:M:207:LYS:HE2	3:Q:191:PRO:HG3	1.02	0.99
1:B:58:GLN:HE21	1:B:58:GLN:N	1.60	0.99
2:M:59:LYS:HG2	2:M:59:LYS:O	1.61	0.99
1:a:243:LEU:CD1	1:b:267:ARG:CD	2.38	0.99
1:a:252:ARG:HB2	1:a:257:LEU:HD22	1.42	0.98
2:m:166:ASP:HB3	2:m:170:GLY:H	1.25	0.98
1:b:277:TRP:CA	1:b:278:THR:HB	1.94	0.97
1:a:263:LEU:C	1:a:263:LEU:CD1	2.30	0.97
3:Q:41:PRO:CD	4:Q:301:HOH:O	2.00	0.96
2:m:59:LYS:O	2:m:59:LYS:HD3	1.62	0.96
2:m:116:ALA:O	2:m:120:PRO:HD2	1.65	0.96
2:m:170:GLY:HA2	2:m:173:GLY:H	1.27	0.96
2:m:166:ASP:CG	2:m:177:LYS:NZ	2.23	0.96
1:B:147:ARG:NH2	4:B:302:HOH:O	1.98	0.96
2:M:207:LYS:CE	3:Q:191:PRO:CG	2.43	0.96
3:q:56:LEU:HD11	4:q:314:HOH:O	1.64	0.96
2:M:207:LYS:NZ	3:Q:191:PRO:CG	2.28	0.96
1:b:96:ALA:HB1	1:b:138:THR:HG21	1.47	0.95
2:m:171:PHE:CD2	2:m:171:PHE:N	2.30	0.95
1:A:263:LEU:HD12	1:A:264:PRO:N	1.81	0.94
2:m:166:ASP:OD1	2:m:167:PRO:HD2	1.67	0.94
3:q:56:LEU:HD11	4:q:318:HOH:O	1.68	0.94
1:A:262:PRO:O	1:A:263:LEU:HB2	1.67	0.93
1:B:101:GLU:HB3	3:Q:215:VAL:HG13	1.49	0.93
1:a:278:THR:O	1:b:278:THR:OG1	1.86	0.93
3:q:25:LEU:CD2	3:q:230:ILE:HD11	1.97	0.93
1:A:98:THR:HG22	1:A:101:GLU:HB2	1.50	0.92
1:B:102:ASP:OD1	4:B:301:HOH:O	1.86	0.92
1:A:97:THR:CG2	2:M:207:LYS:HA	2.00	0.91
2:m:171:PHE:H	2:m:171:PHE:HD2	1.05	0.91
1:A:215:THR:OG1	4:A:301:HOH:O	1.89	0.91
1:b:261:ALA:HB1	1:b:262:PRO:HA	1.53	0.91
1:A:98:THR:HG23	1:A:101:GLU:CB	1.98	0.90
2:m:59:LYS:H	2:m:59:LYS:CD	1.80	0.90
3:q:56:LEU:CD1	4:q:314:HOH:O	2.15	0.90
1:B:101:GLU:HB3	3:Q:215:VAL:CG1	2.02	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:62:SER:O	3:Q:175:ARG:NH2	2.05	0.90
3:q:228:GLY:O	3:q:231:LEU:HD23	1.70	0.90
1:A:98:THR:CG2	1:A:101:GLU:CG	2.50	0.89
2:M:169:SER:OG	2:M:173:GLY:HA3	1.71	0.89
3:q:67:SER:O	4:q:301:HOH:O	1.87	0.89
1:a:259:PRO:O	1:a:259:PRO:HG2	1.70	0.89
1:a:263:LEU:HD13	1:a:264:PRO:C	1.97	0.89
2:m:60:ILE:HD11	3:q:182:THR:OG1	1.72	0.88
1:A:263:LEU:CD1	1:A:264:PRO:N	2.37	0.88
1:a:263:LEU:HD22	1:a:265:LYS:CB	2.04	0.88
2:m:66:SER:HB2	2:m:185:THR:HG23	1.55	0.88
1:a:252:ARG:CB	1:a:257:LEU:HD22	2.04	0.88
1:B:225:GLU:HG3	1:B:226:ALA:N	1.89	0.87
1:a:256:LEU:N	1:a:256:LEU:HD12	1.89	0.87
1:A:109:ASN:O	3:Q:177:ARG:NH1	2.06	0.87
1:b:101:GLU:HB3	3:q:215:VAL:CG1	2.05	0.87
2:m:59:LYS:C	2:m:60:ILE:HD13	1.99	0.87
2:m:166:ASP:CG	2:m:177:LYS:HZ3	1.81	0.87
1:a:243:LEU:HD21	1:b:247:LEU:HD12	1.56	0.86
1:B:261:ALA:CB	1:B:262:PRO:HD2	1.97	0.86
3:q:59:ARG:N	4:q:305:HOH:O	2.05	0.86
3:q:202:THR:OG1	4:q:302:HOH:O	1.91	0.86
1:a:252:ARG:HD2	1:a:257:LEU:HD23	1.56	0.86
2:m:71:THR:O	2:m:73:THR:N	2.07	0.86
1:a:198:HIS:O	1:a:198:HIS:CD2	2.29	0.86
1:a:198:HIS:O	1:a:198:HIS:CG	2.30	0.85
3:Q:229:LEU:O	4:Q:303:HOH:O	1.93	0.85
1:a:263:LEU:HD13	1:a:264:PRO:CA	2.06	0.85
3:Q:55:PHE:HA	4:Q:308:HOH:O	1.75	0.85
3:Q:234:GLN:OE1	4:Q:302:HOH:O	1.93	0.85
1:A:263:LEU:HD13	1:A:264:PRO:HD2	1.59	0.85
2:M:207:LYS:NZ	3:Q:191:PRO:HD3	1.92	0.85
2:m:170:GLY:HA2	2:m:173:GLY:N	1.92	0.84
1:A:139:HIS:CE1	2:M:207:LYS:HG3	2.13	0.84
3:q:76:LEU:N	4:q:306:HOH:O	2.09	0.84
1:a:263:LEU:CD2	1:a:265:LYS:HB3	2.08	0.83
1:a:277:TRP:HB3	1:b:278:THR:HG21	0.86	0.83
1:A:98:THR:CG2	1:A:101:GLU:CD	2.51	0.83
1:A:256:LEU:CD2	1:B:278:THR:O	2.25	0.83
1:A:139:HIS:NE2	2:M:207:LYS:HG3	1.93	0.83
2:M:169:SER:OG	2:M:173:GLY:CA	2.27	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:87:ILE:HD11	3:Q:92:ILE:HG22	1.59	0.83
1:a:258:ALA:HB1	1:a:259:PRO:CD	2.09	0.83
1:b:96:ALA:CB	1:b:138:THR:HG21	2.09	0.83
2:m:53:PHE:O	2:m:56:SER:OG	1.96	0.83
1:A:97:THR:O	1:A:137:PRO:HA	1.77	0.83
1:a:263:LEU:HD11	1:a:264:PRO:O	1.78	0.83
1:b:101:GLU:HB3	3:q:215:VAL:HG13	1.61	0.83
2:m:43:MET:SD	3:q:210:GLN:NE2	2.50	0.83
1:A:117:ALA:O	1:A:121:VAL:HG23	1.77	0.82
3:Q:225:ARG:NH2	4:Q:307:HOH:O	2.13	0.82
1:b:96:ALA:C	1:b:97:THR:HG23	2.00	0.82
3:Q:40:PHE:CA	4:Q:301:HOH:O	2.26	0.82
1:a:263:LEU:HD22	1:a:265:LYS:HB3	1.62	0.82
1:A:98:THR:HG21	1:A:101:GLU:CG	2.09	0.82
2:m:2:HIS:ND1	2:m:102:HIS:CD2	2.48	0.82
1:A:279:ARG:HG3	1:A:279:ARG:HH21	0.73	0.81
2:M:71:THR:O	2:M:73:THR:N	2.13	0.81
1:A:97:THR:O	1:A:138:THR:N	2.13	0.81
3:q:233:LEU:C	3:q:233:LEU:CD2	2.50	0.81
3:Q:209:TRP:HB3	4:Q:305:HOH:O	1.78	0.81
3:Q:211:GLY:O	4:Q:305:HOH:O	1.98	0.81
3:q:25:LEU:HB3	3:q:230:ILE:HD13	1.61	0.81
1:A:264:PRO:O	1:A:265:LYS:HB2	1.79	0.81
1:a:116:GLU:OE2	4:a:301:HOH:O	1.96	0.81
1:A:113:SER:O	1:A:114:GLU:CB	2.28	0.81
3:Q:52:ALA:O	3:Q:56:LEU:N	2.14	0.81
2:m:169:SER:HB2	3:q:88:GLY:HA2	1.63	0.80
3:q:52:ALA:O	3:q:56:LEU:N	2.12	0.80
1:A:112:LEU:HD12	1:A:116:GLU:HB3	1.63	0.80
2:M:116:ALA:O	2:M:120:PRO:CD	2.30	0.80
1:b:71:HIS:ND1	1:b:71:HIS:N	2.30	0.80
1:a:263:LEU:O	1:a:265:LYS:CB	2.30	0.80
2:m:166:ASP:OD1	2:m:167:PRO:CD	2.30	0.80
1:b:257:LEU:HD21	1:b:273:GLN:NE2	1.95	0.80
1:a:231:ARG:O	4:a:302:HOH:O	1.99	0.80
1:a:263:LEU:CD1	1:a:264:PRO:O	2.30	0.79
1:a:265:LYS:HG3	1:a:266:THR:HG23	1.65	0.79
1:a:265:LYS:O	1:a:265:LYS:CD	2.30	0.79
3:q:25:LEU:HB3	3:q:230:ILE:CD1	2.12	0.79
1:B:178:GLN:OE1	4:B:303:HOH:O	1.99	0.79
1:a:252:ARG:CA	1:a:257:LEU:HD22	2.11	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:ARG:HH21	1:B:249:LEU:HB2	1.46	0.79
2:m:116:ALA:O	2:m:120:PRO:CD	2.29	0.79
1:a:258:ALA:HB1	1:a:259:PRO:HD2	1.65	0.79
2:M:207:LYS:NZ	3:Q:191:PRO:CD	2.45	0.79
1:a:263:LEU:HD13	1:a:263:LEU:O	1.82	0.79
3:q:25:LEU:CG	3:q:230:ILE:CD1	2.61	0.79
2:m:153:TYR:OH	2:m:179:GLY:O	1.99	0.79
1:A:113:SER:O	1:A:114:GLU:HB3	1.82	0.78
1:a:263:LEU:HD22	1:a:263:LEU:O	1.82	0.78
1:a:279:ARG:NH1	1:b:276:GLY:O	2.16	0.78
2:M:207:LYS:HZ3	3:Q:191:PRO:CG	1.93	0.78
2:M:64:THR:OG1	2:M:188:PRO:CB	2.30	0.78
1:B:22:ASP:O	1:B:217:ARG:NH1	2.17	0.78
1:a:259:PRO:O	1:a:260:GLU:HB2	1.82	0.78
1:b:255:GLY:O	1:b:256:LEU:HD23	1.83	0.78
1:b:72:SER:O	1:b:75:ASP:HB2	1.82	0.78
1:B:19:LYS:O	4:B:304:HOH:O	2.01	0.78
3:Q:66:ALA:O	3:Q:70:VAL:HG23	1.84	0.78
1:a:244:VAL:HG13	1:a:270:LEU:HD13	1.64	0.78
1:A:279:ARG:O	1:A:280:ARG:HB2	1.82	0.77
1:a:256:LEU:N	1:a:256:LEU:CD1	2.46	0.77
2:m:62:SER:HB2	2:m:64:THR:H	1.50	0.77
3:q:25:LEU:CG	3:q:230:ILE:HD11	2.14	0.77
2:M:115:MET:O	2:M:120:PRO:HD2	1.84	0.77
1:A:36:ILE:HG12	1:A:196:SER:HA	1.66	0.77
1:A:112:LEU:CD1	1:A:116:GLU:HB3	2.14	0.77
1:B:261:ALA:HB1	1:B:262:PRO:CD	2.13	0.77
1:A:263:LEU:HD13	1:A:264:PRO:CD	2.15	0.77
3:q:25:LEU:HG	3:q:230:ILE:CD1	2.14	0.77
3:Q:87:ILE:HD11	3:Q:92:ILE:CG2	2.12	0.77
3:q:198:ARG:NH1	4:q:303:HOH:O	1.92	0.76
1:a:248:ALA:HB1	1:a:264:PRO:HG2	1.67	0.76
1:A:262:PRO:O	1:A:263:LEU:CB	2.30	0.76
1:A:98:THR:HG22	1:A:101:GLU:CD	2.09	0.76
1:a:259:PRO:O	1:a:259:PRO:CG	2.30	0.76
1:a:263:LEU:O	1:a:265:LYS:HB2	1.84	0.76
1:A:231:ARG:NH2	1:A:246:ASP:OD1	2.17	0.76
3:Q:55:PHE:CA	4:Q:308:HOH:O	2.32	0.76
1:a:266:THR:OG1	1:a:268:ASP:HB2	1.84	0.76
1:b:96:ALA:HB1	1:b:138:THR:CG2	2.14	0.76
2:m:166:ASP:HB3	2:m:170:GLY:N	1.99	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:166:ASP:OD2	3:q:87:ILE:HG22	1.84	0.75
1:a:157:MET:HE1	3:q:170:LEU:HG	1.66	0.75
1:b:178:GLN:OE1	4:b:301:HOH:O	2.04	0.75
1:b:70:GLY:O	1:b:75:ASP:CB	2.34	0.75
1:A:97:THR:HG21	2:M:206:GLY:C	2.12	0.75
1:B:23:ASP:O	1:B:217:ARG:NH1	2.19	0.75
2:m:6:GLY:O	2:m:7:TYR:CB	2.31	0.75
3:q:198:ARG:HD2	4:q:303:HOH:O	1.86	0.74
1:B:147:ARG:CZ	4:B:302:HOH:O	2.33	0.74
2:M:2:HIS:CE1	2:M:102:HIS:HD2	2.05	0.74
2:m:166:ASP:CG	2:m:177:LYS:HZ1	1.94	0.74
1:b:278:THR:CG2	1:b:279:ARG:N	2.30	0.74
1:a:116:GLU:CD	4:a:301:HOH:O	2.30	0.74
1:A:98:THR:HG21	1:A:101:GLU:CD	2.13	0.74
2:M:100:LEU:O	2:M:101:ALA:HB3	1.88	0.73
1:B:277:TRP:O	1:B:278:THR:CG2	2.30	0.73
2:m:116:ALA:O	2:m:120:PRO:HG2	1.89	0.73
3:Q:40:PHE:HB3	4:Q:301:HOH:O	1.87	0.73
1:B:19:LYS:CB	4:B:304:HOH:O	2.36	0.73
1:a:263:LEU:O	1:a:264:PRO:C	2.29	0.73
1:A:141:LEU:HB3	1:A:145:GLN:HG3	1.71	0.73
2:M:4:MET:HE3	3:Q:75:PHE:CD2	2.23	0.73
1:B:147:ARG:NE	4:B:302:HOH:O	2.21	0.72
3:q:208:ASN:O	3:q:209:TRP:C	2.29	0.72
2:M:177:LYS:HZ3	3:Q:86:GLN:HA	1.54	0.72
1:A:139:HIS:NE2	4:A:302:HOH:O	2.21	0.72
3:Q:87:ILE:CD1	3:Q:92:ILE:HG23	2.18	0.72
1:a:244:VAL:HG13	1:a:270:LEU:HD12	1.71	0.72
2:m:102:HIS:CE1	4:m:302:HOH:O	2.42	0.71
3:q:25:LEU:HD23	3:q:230:ILE:CD1	2.17	0.71
1:a:4:ILE:HD12	1:a:30:LYS:HG3	1.73	0.71
1:a:251:ALA:HB1	1:a:256:LEU:HB2	1.72	0.71
1:b:96:ALA:O	1:b:97:THR:CG2	2.30	0.71
1:b:277:TRP:HA	1:b:278:THR:CB	2.15	0.71
2:M:59:LYS:O	2:M:59:LYS:CG	2.30	0.71
3:q:74:GLY:O	3:q:78:THR:HG23	1.90	0.71
1:A:97:THR:HG21	2:M:206:GLY:O	1.91	0.71
3:Q:225:ARG:CZ	4:Q:307:HOH:O	2.38	0.71
1:a:116:GLU:OE1	4:a:301:HOH:O	2.09	0.70
3:Q:71:LEU:N	3:Q:72:PRO:CD	2.53	0.70
1:b:72:SER:O	1:b:75:ASP:N	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:PRO:O	1:A:265:LYS:CB	2.36	0.70
3:Q:64:PHE:O	3:Q:67:SER:OG	2.09	0.70
1:b:187:ARG:NH2	4:b:303:HOH:O	2.24	0.70
3:Q:201:GLU:OE1	4:Q:306:HOH:O	2.09	0.70
2:M:207:LYS:HZ3	3:Q:191:PRO:CD	2.04	0.69
1:a:263:LEU:HD22	1:a:265:LYS:HB2	1.74	0.69
1:b:96:ALA:C	1:b:97:THR:CG2	2.65	0.69
1:A:98:THR:CG2	1:A:101:GLU:OE1	2.40	0.69
3:q:25:LEU:HG	3:q:230:ILE:HD12	1.74	0.69
1:a:277:TRP:CG	1:b:278:THR:HG21	2.27	0.68
1:B:160:GLU:OE1	4:B:305:HOH:O	2.12	0.68
3:Q:40:PHE:CB	4:Q:301:HOH:O	2.41	0.68
3:Q:232:THR:OG1	3:Q:235:ALA:HB3	1.94	0.68
1:a:243:LEU:CD2	1:b:247:LEU:HD12	2.23	0.68
2:m:116:ALA:O	2:m:120:PRO:CG	2.41	0.68
2:M:115:MET:O	2:M:116:ALA:C	2.30	0.68
1:b:8:GLU:CD	1:b:61:ARG:HH21	2.02	0.68
2:m:167:PRO:CB	3:q:86:GLN:NE2	2.55	0.68
2:m:166:ASP:H	2:m:170:GLY:HA3	1.56	0.68
1:b:148:ARG:CZ	1:b:178:GLN:HE22	2.07	0.67
3:q:133:ARG:HG2	3:q:142:ILE:HD13	1.75	0.67
1:a:252:ARG:CB	1:a:257:LEU:CD2	2.65	0.67
2:m:43:MET:CE	3:q:210:GLN:HE21	2.07	0.67
1:A:279:ARG:O	1:A:280:ARG:CB	2.39	0.67
2:M:207:LYS:HZ1	3:Q:191:PRO:HD3	1.59	0.67
2:M:16:TRP:CZ2	2:M:159:GLN:HG2	2.29	0.67
1:b:261:ALA:HA	1:b:262:PRO:O	1.95	0.66
1:a:265:LYS:O	1:a:265:LYS:CG	2.43	0.66
1:b:101:GLU:HB3	3:q:215:VAL:HG11	1.77	0.66
2:m:100:LEU:O	2:m:101:ALA:HB3	1.94	0.66
1:A:110:LEU:HD23	3:Q:170:LEU:HD11	1.78	0.66
3:q:210:GLN:OE1	3:q:211:GLY:HA2	1.96	0.66
1:B:174:ALA:O	1:B:178:GLN:HG3	1.96	0.66
1:a:263:LEU:CD1	1:a:264:PRO:C	2.67	0.66
2:m:167:PRO:HB2	3:q:86:GLN:HE22	1.60	0.66
2:m:168:ALA:CB	3:q:87:ILE:O	2.39	0.66
1:B:19:LYS:HB2	4:B:304:HOH:O	1.93	0.66
3:Q:87:ILE:HD13	3:Q:92:ILE:HG23	1.73	0.65
1:b:277:TRP:CB	1:b:278:THR:HB	2.26	0.65
2:m:115:MET:O	2:m:120:PRO:HD2	1.96	0.65
3:q:25:LEU:CB	3:q:230:ILE:CD1	2.74	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:THR:CG2	4:A:301:HOH:O	2.43	0.65
3:q:210:GLN:OE1	3:q:211:GLY:N	2.29	0.65
3:q:228:GLY:HA2	3:q:231:LEU:HD22	1.78	0.65
2:M:166:ASP:HB2	2:M:177:LYS:HZ2	1.61	0.65
2:M:177:LYS:NZ	3:Q:86:GLN:HA	2.11	0.65
1:b:214:ARG:HG3	1:b:237:VAL:HG12	1.79	0.65
1:a:105:PHE:HD2	3:q:169:ARG:HD3	1.62	0.65
1:a:250:LEU:C	1:a:252:ARG:N	2.53	0.65
2:M:207:LYS:HZ3	3:Q:191:PRO:HD3	1.59	0.64
1:A:97:THR:HG22	2:M:207:LYS:HA	1.77	0.64
1:A:98:THR:HG23	1:A:101:GLU:H	1.61	0.64
3:Q:136:ARG:N	4:Q:304:HOH:O	1.98	0.64
1:a:263:LEU:CD1	1:a:264:PRO:N	2.54	0.64
2:M:166:ASP:OD1	2:M:169:SER:N	2.30	0.64
1:A:56:ARG:NH2	4:A:306:HOH:O	2.29	0.64
1:a:252:ARG:HA	1:a:257:LEU:HD22	1.79	0.64
1:b:259:PRO:O	1:b:260:GLU:HB3	1.96	0.63
1:A:187:ARG:NH2	4:A:304:HOH:O	2.24	0.63
2:M:58:LEU:O	2:M:69:HIS:ND1	2.27	0.63
1:a:151:ILE:O	1:a:155:VAL:HG13	1.98	0.63
1:b:268:ASP:O	1:b:272:ALA:N	2.32	0.63
1:B:96:ALA:HB1	1:B:138:THR:HG21	1.79	0.63
1:b:263:LEU:HD12	1:b:264:PRO:HD2	1.81	0.63
1:A:98:THR:HG22	1:A:101:GLU:CB	2.17	0.63
1:a:250:LEU:C	1:a:252:ARG:H	2.07	0.63
3:q:118:PHE:O	3:q:122:THR:HG21	1.95	0.63
2:M:177:LYS:HE2	3:Q:87:ILE:CB	2.29	0.62
1:A:47:LEU:HD22	1:A:213:PHE:HZ	1.63	0.62
2:M:64:THR:OG1	2:M:188:PRO:HB3	1.99	0.62
1:B:4:ILE:HD12	1:B:30:LYS:HG3	1.82	0.62
2:M:64:THR:OG1	2:M:188:PRO:CG	2.47	0.62
2:M:173:GLY:O	2:M:177:LYS:HG3	2.00	0.62
1:b:280:ARG:HD2	1:b:280:ARG:O	1.99	0.62
2:m:6:GLY:O	2:m:7:TYR:HB2	1.99	0.62
1:B:278:THR:HG23	1:B:279:ARG:H	1.61	0.62
1:A:109:ASN:HB3	3:Q:170:LEU:HB2	1.81	0.62
3:q:169:ARG:NH2	4:q:307:HOH:O	2.31	0.62
1:b:256:LEU:O	1:b:277:TRP:NE1	2.31	0.61
1:B:118:ARG:O	1:B:122:GLU:HG2	1.99	0.61
1:a:256:LEU:CD1	1:a:256:LEU:H	2.13	0.61
1:B:180:LEU:HB3	1:B:184:ARG:NH1	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:59:LYS:O	2:m:60:ILE:CD1	2.41	0.61
1:A:98:THR:HG21	1:A:101:GLU:HG3	1.80	0.61
3:Q:209:TRP:CB	4:Q:305:HOH:O	2.43	0.61
3:q:74:GLY:N	4:q:306:HOH:O	2.34	0.61
1:A:197:THR:OG1	1:A:198:HIS:N	2.33	0.61
1:b:4:ILE:HD11	1:b:160:GLU:HB3	1.82	0.61
1:a:248:ALA:CB	1:a:264:PRO:HG2	2.29	0.61
1:a:263:LEU:HD21	1:a:265:LYS:HB3	1.83	0.61
3:q:71:LEU:HD23	4:q:301:HOH:O	2.00	0.61
1:A:97:THR:CG2	2:M:207:LYS:CA	2.77	0.61
1:A:113:SER:O	1:A:114:GLU:CG	2.49	0.61
1:A:263:LEU:HD13	1:A:264:PRO:N	2.15	0.60
3:Q:68:VAL:O	3:Q:71:LEU:CD1	2.42	0.60
1:A:147:ARG:NH1	1:A:167:PRO:O	2.35	0.60
1:A:271:ALA:HB2	1:B:250:LEU:HD21	1.84	0.60
3:Q:71:LEU:N	3:Q:72:PRO:HD2	2.16	0.60
1:a:252:ARG:HB2	1:a:257:LEU:HD23	1.79	0.60
1:A:279:ARG:HG2	1:B:278:THR:CG2	2.31	0.60
2:M:166:ASP:HB2	2:M:177:LYS:NZ	2.17	0.60
1:a:118:ARG:O	1:a:122:GLU:HG3	2.01	0.60
1:a:250:LEU:O	1:a:252:ARG:N	2.35	0.60
1:b:164:LEU:HB3	1:b:167:PRO:HG3	1.82	0.60
1:a:24:LEU:HD11	1:a:213:PHE:CZ	2.35	0.60
1:a:274:MET:HB2	1:a:277:TRP:CZ3	2.36	0.60
1:A:97:THR:O	1:A:137:PRO:CA	2.50	0.60
1:A:118:ARG:CZ	1:A:134:ARG:NH2	2.64	0.60
3:q:226:VAL:CG2	4:q:304:HOH:O	2.33	0.60
1:A:56:ARG:HG3	1:A:71:HIS:CE1	2.37	0.60
1:B:98:THR:OG1	1:B:101:GLU:CG	2.40	0.60
1:a:274:MET:HB2	1:a:277:TRP:CE3	2.36	0.60
1:B:93:GLN:HB2	3:Q:207:ARG:HH12	1.66	0.60
2:M:207:LYS:HZ1	3:Q:191:PRO:CD	2.13	0.59
1:a:258:ALA:CB	1:a:259:PRO:CD	2.78	0.59
3:q:68:VAL:C	4:q:301:HOH:O	2.45	0.59
2:m:173:GLY:O	2:m:177:LYS:HG3	2.01	0.59
1:B:231:ARG:HH21	1:B:249:LEU:CB	2.16	0.59
2:m:16:TRP:CZ2	2:m:159:GLN:HG2	2.37	0.59
1:A:97:THR:HG21	2:M:207:LYS:HA	1.84	0.59
1:A:279:ARG:HB2	1:B:276:GLY:O	2.03	0.59
1:b:4:ILE:HD12	1:b:30:LYS:HG3	1.85	0.59
2:m:1:MET:HG2	2:m:186:GLN:NE2	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ARG:HG2	1:B:215:THR:HG23	1.85	0.58
2:m:42:ARG:CZ	3:q:211:GLY:O	2.51	0.58
1:A:243:LEU:HD23	1:B:243:LEU:HG	1.84	0.58
2:M:3:ILE:HG21	2:M:8:LEU:HD13	1.85	0.58
1:b:67:THR:HG23	4:b:312:HOH:O	2.02	0.58
1:B:277:TRP:C	1:B:278:THR:HG22	2.27	0.58
3:Q:135:TRP:CA	4:Q:304:HOH:O	2.51	0.58
1:b:91:ASP:OD1	3:q:150:ARG:NH2	2.36	0.58
1:a:259:PRO:O	1:a:260:GLU:CB	2.52	0.58
2:m:166:ASP:OD1	2:m:167:PRO:N	2.36	0.58
3:q:5:SER:OG	3:q:6:ILE:N	2.37	0.58
1:A:130:ILE:HB	1:A:133:LEU:HD12	1.85	0.58
1:A:174:ALA:O	1:A:178:GLN:HG3	2.03	0.58
1:a:265:LYS:C	1:a:266:THR:HG23	2.29	0.58
1:b:21:LEU:HD22	1:b:24:LEU:HD13	1.85	0.58
2:m:59:LYS:CD	2:m:59:LYS:N	2.49	0.58
1:b:252:ARG:O	1:b:252:ARG:NE	2.37	0.58
1:A:157:MET:HE1	3:Q:170:LEU:HG	1.85	0.58
1:A:214:ARG:HB2	1:A:237:VAL:HG12	1.86	0.58
1:B:96:ALA:CB	1:B:138:THR:HG21	2.33	0.58
3:q:198:ARG:O	3:q:201:GLU:HB3	2.03	0.58
3:q:210:GLN:OE1	3:q:211:GLY:CA	2.52	0.58
3:q:51:LEU:O	3:q:55:PHE:HD1	1.88	0.57
3:q:86:GLN:HE22	3:q:96:PRO:HD2	1.69	0.57
3:q:226:VAL:CA	4:q:304:HOH:O	2.46	0.57
1:a:106:GLY:HA3	1:a:157:MET:HG3	1.87	0.57
2:m:59:LYS:HD2	2:m:59:LYS:N	2.04	0.57
1:a:112:LEU:HB3	1:a:116:GLU:HB3	1.86	0.57
1:B:96:ALA:HB1	1:B:138:THR:CG2	2.35	0.57
1:b:277:TRP:HB3	1:b:278:THR:HB	1.87	0.57
3:q:25:LEU:CB	3:q:230:ILE:HD11	2.35	0.57
2:M:4:MET:HE3	3:Q:75:PHE:HD2	1.68	0.57
2:M:103:GLY:HA3	4:M:302:HOH:O	2.05	0.57
1:A:113:SER:O	1:A:114:GLU:CD	2.48	0.56
1:A:118:ARG:NH1	1:A:134:ARG:HH21	2.02	0.56
3:Q:225:ARG:NH1	4:Q:307:HOH:O	2.37	0.56
1:b:35:ALA:HB3	1:b:210:VAL:HG22	1.87	0.56
2:m:62:SER:OG	2:m:64:THR:O	2.21	0.56
1:A:279:ARG:CB	1:B:276:GLY:O	2.53	0.56
1:B:134:ARG:HG3	1:B:135:ASP:OD1	2.06	0.56
1:B:244:VAL:HG23	4:B:313:HOH:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:263:LEU:CD2	1:a:265:LYS:CB	2.75	0.56
1:b:47:LEU:HD22	1:b:213:PHE:HZ	1.70	0.56
2:m:115:MET:O	2:m:120:PRO:CD	2.52	0.56
3:q:41:PRO:HG2	3:q:241:GLY:HA2	1.86	0.56
1:A:36:ILE:CG1	1:A:196:SER:HA	2.35	0.56
1:a:265:LYS:O	1:a:266:THR:CG2	2.53	0.56
1:A:110:LEU:CD2	3:Q:170:LEU:HD11	2.35	0.56
1:A:139:HIS:CE1	4:A:302:HOH:O	2.59	0.56
3:Q:198:ARG:O	3:Q:201:GLU:HB3	2.06	0.56
1:A:47:LEU:HD22	1:A:213:PHE:CZ	2.41	0.56
1:b:157:MET:O	1:b:159:PRO:HD3	2.06	0.56
2:m:176:LEU:O	2:m:180:SER:OG	2.22	0.56
3:q:223:SER:O	3:q:227:LEU:HB2	2.05	0.56
1:A:110:LEU:HD23	3:Q:170:LEU:CD1	2.36	0.56
1:a:243:LEU:HD13	1:b:267:ARG:HD3	1.79	0.56
1:a:266:THR:C	1:a:268:ASP:N	2.58	0.56
1:b:97:THR:O	1:b:98:THR:HG22	2.05	0.56
1:b:166:GLU:N	1:b:167:PRO:HD3	2.20	0.56
1:a:263:LEU:O	1:a:265:LYS:N	2.39	0.56
1:a:271:ALA:HB2	1:b:250:LEU:HD21	1.87	0.56
3:Q:239:ALA:HA	3:Q:242:VAL:HG12	1.89	0.55
1:A:120:ARG:O	1:A:123:GLU:HG2	2.06	0.55
2:M:169:SER:HB3	3:Q:87:ILE:O	2.06	0.55
1:b:214:ARG:HD3	1:b:219:LEU:HD21	1.88	0.55
3:q:63:ARG:HG2	3:q:64:PHE:N	2.19	0.55
3:q:64:PHE:O	3:q:67:SER:OG	2.19	0.55
3:Q:70:VAL:O	3:Q:73:LEU:HB3	2.06	0.55
3:Q:135:TRP:CB	4:Q:304:HOH:O	2.29	0.55
1:b:257:LEU:HD21	1:b:273:GLN:HE22	1.72	0.55
3:q:72:PRO:O	3:q:73:LEU:HB2	2.05	0.55
1:A:113:SER:O	1:A:114:GLU:OE2	2.25	0.55
3:q:174:THR:OG1	3:q:177:ARG:HB2	2.07	0.55
3:q:236:ALA:O	3:q:240:ALA:N	2.36	0.55
2:m:170:GLY:HA2	2:m:171:PHE:C	2.31	0.55
2:m:174:ALA:HA	2:m:177:LYS:HE3	1.87	0.55
1:a:243:LEU:CD1	1:b:267:ARG:CG	2.84	0.55
1:b:92:ASP:OD2	4:b:302:HOH:O	2.18	0.55
1:a:197:THR:HB	1:a:202:LEU:HD23	1.89	0.55
2:m:43:MET:HE3	3:q:201:GLU:HB2	1.89	0.55
2:m:43:MET:HE1	3:q:210:GLN:HE21	1.72	0.55
1:a:178:GLN:O	1:a:182:LEU:HD13	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:LEU:HD21	1:B:151:ILE:HB	1.89	0.54
1:a:158:ARG:N	1:a:159:PRO:HD3	2.22	0.54
1:B:19:LYS:C	4:B:304:HOH:O	2.46	0.54
1:b:180:LEU:HB3	1:b:184:ARG:NH1	2.22	0.54
1:a:277:TRP:CG	1:b:278:THR:CG2	2.90	0.54
3:q:207:ARG:O	3:q:208:ASN:HB2	2.05	0.54
1:b:257:LEU:CD2	1:b:273:GLN:NE2	2.68	0.54
3:q:45:LEU:HB3	3:q:237:ILE:HD13	1.89	0.54
1:B:225:GLU:HG3	1:B:226:ALA:H	1.71	0.54
2:m:166:ASP:CB	2:m:177:LYS:HZ1	2.19	0.54
1:B:38:GLY:O	1:B:44:LYS:NZ	2.36	0.54
2:M:2:HIS:ND1	2:M:102:HIS:HD2	2.05	0.54
3:Q:23:LYS:HE2	3:Q:123:THR:OG1	2.07	0.54
2:m:63:VAL:O	2:m:64:THR:HG23	2.06	0.54
3:Q:166:GLN:HG2	3:Q:181:SER:OG	2.08	0.54
1:B:86:VAL:HA	1:B:93:GLN:HE22	1.73	0.54
3:Q:73:LEU:CD1	3:Q:74:GLY:N	2.69	0.53
2:m:118:VAL:O	2:m:119:GLY:C	2.46	0.53
2:m:171:PHE:N	2:m:171:PHE:HD2	1.85	0.53
1:B:63:LEU:HD23	1:B:68:ALA:HA	1.90	0.53
2:M:193:GLU:O	2:M:197:THR:HG23	2.07	0.53
1:a:266:THR:C	1:a:268:ASP:H	2.16	0.53
1:B:180:LEU:HD22	1:B:184:ARG:HH12	1.71	0.53
3:q:25:LEU:CD2	3:q:230:ILE:CD1	2.77	0.53
2:M:100:LEU:O	2:M:101:ALA:CB	2.53	0.53
2:M:114:SER:O	2:M:115:MET:C	2.46	0.53
1:B:96:ALA:O	1:B:97:THR:HB	2.09	0.53
1:a:258:ALA:CB	1:a:259:PRO:HD2	2.38	0.53
1:a:271:ALA:CB	1:b:250:LEU:HD21	2.39	0.53
1:a:102:ASP:OD2	3:q:169:ARG:NH2	2.41	0.53
1:a:103:VAL:HG21	1:a:125:LEU:HD21	1.90	0.53
2:m:106:THR:HG21	3:q:35:VAL:HG21	1.90	0.53
1:a:252:ARG:HA	1:a:257:LEU:HB2	1.92	0.52
1:A:1:MET:C	1:A:3:PRO:HD2	2.34	0.52
1:A:112:LEU:HD13	1:A:116:GLU:HB3	1.91	0.52
1:B:58:GLN:HE21	1:B:58:GLN:CA	2.21	0.52
2:M:64:THR:OG1	2:M:188:PRO:HG2	2.10	0.52
3:q:236:ALA:O	3:q:239:ALA:N	2.39	0.52
1:a:265:LYS:O	1:a:265:LYS:HG3	2.10	0.52
1:b:271:ALA:HA	1:b:274:MET:HG3	1.91	0.52
1:B:58:GLN:N	1:B:58:GLN:NE2	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:263:LEU:CD1	1:b:264:PRO:HD2	2.40	0.52
1:B:133:LEU:HD22	1:B:136:ARG:HD3	1.92	0.52
1:A:278:THR:HG23	1:A:278:THR:O	2.09	0.52
3:Q:232:THR:HA	3:Q:235:ALA:H	1.75	0.52
2:m:62:SER:CB	2:m:64:THR:H	2.21	0.52
3:q:86:GLN:NE2	3:q:96:PRO:HD2	2.25	0.51
2:M:2:HIS:ND1	2:M:102:HIS:CD2	2.78	0.51
3:Q:86:GLN:OE1	3:Q:96:PRO:HD3	2.10	0.51
3:q:34:ALA:O	3:q:108:ARG:HG3	2.11	0.51
3:Q:71:LEU:CD1	3:Q:71:LEU:N	2.30	0.51
1:a:20:ALA:O	1:a:21:LEU:HD23	2.11	0.51
1:A:256:LEU:HD21	1:B:278:THR:O	2.09	0.51
1:A:279:ARG:HB2	1:B:277:TRP:HA	1.93	0.51
1:a:195:PHE:N	1:a:195:PHE:CD2	2.78	0.51
1:A:127:ALA:O	1:A:182:LEU:HD22	2.11	0.51
1:a:136:ARG:NH2	1:a:141:LEU:HD23	2.26	0.51
1:A:1:MET:N	4:A:310:HOH:O	2.45	0.50
1:a:278:THR:HG22	1:b:280:ARG:HA	1.93	0.50
2:m:71:THR:H	2:m:193:GLU:CD	2.19	0.50
1:B:77:THR:HG23	3:Q:208:ASN:HD21	1.76	0.50
2:M:59:LYS:HG3	3:Q:178:TRP:HE1	1.76	0.50
3:Q:76:LEU:O	3:Q:76:LEU:HD23	2.12	0.50
3:Q:232:THR:O	3:Q:236:ALA:N	2.44	0.50
1:b:98:THR:OG1	1:b:101:GLU:HG3	2.11	0.50
3:q:71:LEU:HG	3:q:72:PRO:HD3	1.92	0.50
1:A:82:ARG:NE	1:A:160:GLU:OE2	2.34	0.50
1:a:128:LEU:HD21	1:a:151:ILE:HB	1.93	0.50
1:b:180:LEU:HD22	1:b:184:ARG:HH12	1.76	0.50
2:m:196:LEU:HD12	3:q:183:ALA:HB2	1.94	0.50
2:M:66:SER:OG	2:M:67:CYS:N	2.43	0.50
2:m:100:LEU:O	2:m:101:ALA:CB	2.59	0.50
1:A:279:ARG:NH2	1:A:279:ARG:CG	2.35	0.50
3:q:199:ARG:NH2	4:q:308:HOH:O	2.34	0.50
1:b:260:GLU:HG3	1:b:261:ALA:O	2.12	0.50
2:m:193:GLU:O	2:m:197:THR:HG23	2.11	0.50
3:Q:73:LEU:HB2	4:Q:314:HOH:O	2.12	0.50
3:Q:167:ARG:O	3:Q:169:ARG:O	2.29	0.50
1:a:256:LEU:H	1:a:256:LEU:HD13	1.76	0.50
1:b:255:GLY:C	1:b:256:LEU:HD23	2.37	0.49
2:M:2:HIS:CE1	2:M:102:HIS:CD2	2.93	0.49
2:m:102:HIS:O	2:m:103:GLY:O	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:SER:C	1:A:114:GLU:CG	2.85	0.49
1:A:114:GLU:HG2	1:A:115:ALA:H	1.77	0.49
1:A:133:LEU:HD11	1:A:145:GLN:HE21	1.77	0.49
2:m:8:LEU:O	2:m:9:PRO:O	2.29	0.49
2:m:112:ALA:O	2:m:113:PHE:C	2.50	0.49
1:B:101:GLU:HB3	3:Q:215:VAL:HG11	1.91	0.49
1:a:277:TRP:HE3	1:b:256:LEU:HD13	1.78	0.49
1:A:32:GLU:O	1:A:192:THR:HG23	2.12	0.49
1:b:72:SER:O	1:b:75:ASP:CB	2.59	0.49
1:B:73:ARG:N	1:B:73:ARG:HD2	2.28	0.49
3:q:191:PRO:O	3:q:195:THR:HG23	2.13	0.49
2:M:68:SER:HB2	2:M:189:LEU:HD13	1.95	0.49
2:M:115:MET:O	2:M:116:ALA:O	2.30	0.49
2:m:174:ALA:HA	2:m:177:LYS:CE	2.43	0.49
1:A:168:THR:HA	1:A:171:LEU:HD12	1.95	0.49
3:Q:163:THR:O	3:Q:167:ARG:HG3	2.13	0.48
2:m:5:GLU:OE1	2:m:5:GLU:O	2.30	0.48
2:m:62:SER:C	2:m:64:THR:H	2.20	0.48
1:B:23:ASP:C	1:B:217:ARG:HH12	2.14	0.48
2:M:177:LYS:CE	3:Q:87:ILE:HB	2.43	0.48
1:a:105:PHE:O	1:a:109:ASN:ND2	2.46	0.48
3:q:208:ASN:O	3:q:209:TRP:O	2.30	0.48
3:q:210:GLN:OE1	3:q:210:GLN:C	2.55	0.48
1:a:263:LEU:CD1	1:a:264:PRO:CA	2.85	0.48
1:b:246:ASP:O	1:b:250:LEU:N	2.45	0.48
3:Q:30:PHE:HD1	3:Q:33:LEU:HD12	1.78	0.48
1:b:279:ARG:O	1:b:280:ARG:C	2.55	0.48
1:a:252:ARG:CD	1:a:257:LEU:HD23	2.36	0.48
1:b:11:THR:HA	1:b:21:LEU:O	2.14	0.48
1:b:97:THR:C	1:b:98:THR:CG2	2.86	0.48
2:m:62:SER:HG	2:m:64:THR:C	2.18	0.48
2:m:66:SER:CB	2:m:185:THR:HG23	2.36	0.48
2:m:148:GLY:O	2:m:152:THR:HG23	2.13	0.48
1:B:128:LEU:HD13	1:B:152:ALA:HA	1.96	0.48
3:Q:88:GLY:O	3:Q:89:PRO:C	2.57	0.48
1:a:262:PRO:O	1:a:263:LEU:HB3	2.13	0.48
3:q:166:GLN:HG2	3:q:181:SER:OG	2.14	0.48
1:A:105:PHE:HD2	3:Q:169:ARG:HD3	1.78	0.48
1:A:136:ARG:HD2	1:A:141:LEU:HD23	1.95	0.48
2:M:28:ALA:HB1	3:Q:141:LEU:HD11	1.96	0.48
1:a:277:TRP:CB	1:b:278:THR:CG2	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:118:ARG:O	1:b:122:GLU:HG2	2.13	0.48
2:m:63:VAL:C	2:m:64:THR:HG23	2.39	0.48
3:q:1:MET:HG2	3:q:3:ILE:HG12	1.95	0.48
3:q:19:PRO:HB3	3:q:222:ALA:HB2	1.96	0.48
1:A:112:LEU:N	1:A:112:LEU:CD2	2.77	0.48
1:B:19:LYS:HB3	4:B:304:HOH:O	2.08	0.48
2:M:116:ALA:O	2:M:120:PRO:CG	2.61	0.48
3:Q:76:LEU:O	3:Q:76:LEU:CD2	2.61	0.48
1:a:265:LYS:O	1:a:266:THR:HG23	2.13	0.48
1:a:265:LYS:C	1:a:266:THR:CG2	2.87	0.48
1:B:157:MET:O	1:B:159:PRO:HD3	2.14	0.47
3:q:58:ALA:CA	4:q:305:HOH:O	2.58	0.47
3:Q:211:GLY:O	3:Q:212:GLU:CB	2.61	0.47
1:a:174:ALA:O	1:a:178:GLN:HG3	2.14	0.47
1:a:258:ALA:HB1	1:a:259:PRO:HD3	1.92	0.47
2:m:119:GLY:N	2:m:120:PRO:HD2	2.29	0.47
2:m:166:ASP:CB	2:m:177:LYS:NZ	2.75	0.47
1:B:91:ASP:OD1	3:Q:150:ARG:NH2	2.48	0.47
3:Q:214:ARG:NH1	4:Q:310:HOH:O	2.45	0.47
1:a:97:THR:O	1:a:137:PRO:HA	2.13	0.47
1:a:121:VAL:O	1:a:125:LEU:HG	2.14	0.47
1:b:122:GLU:CD	1:b:134:ARG:HH22	2.22	0.47
1:A:215:THR:HG21	4:A:301:HOH:O	2.08	0.47
1:a:157:MET:CE	3:q:170:LEU:HG	2.42	0.47
1:B:233:THR:HA	1:B:236:LYS:HD2	1.95	0.47
2:m:1:MET:HG2	2:m:186:GLN:HE22	1.78	0.47
2:m:6:GLY:HA3	3:q:109:ALA:HA	1.96	0.47
2:m:119:GLY:N	2:m:120:PRO:CD	2.74	0.47
1:B:12:TYR:O	1:B:20:ALA:N	2.47	0.47
2:m:2:HIS:CD2	2:m:115:MET:HE3	2.49	0.47
1:B:261:ALA:CB	1:B:262:PRO:CD	2.76	0.47
1:b:64:LEU:HB2	1:b:69:THR:CG2	2.45	0.47
2:m:116:ALA:O	2:m:117:ILE:C	2.55	0.47
1:a:243:LEU:HD12	1:b:267:ARG:CD	2.23	0.47
2:m:8:LEU:C	2:m:9:PRO:O	2.58	0.47
2:m:55:LEU:C	2:m:57:ALA:H	2.22	0.47
1:B:167:PRO:HG2	1:B:202:LEU:HD21	1.96	0.46
1:b:242:PRO:HG2	1:b:245:ILE:HD13	1.97	0.46
2:m:6:GLY:O	2:m:7:TYR:HB3	2.13	0.46
1:A:219:LEU:HD22	1:A:237:VAL:HG13	1.98	0.46
2:M:76:GLY:O	2:M:80:PHE:N	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:196:LEU:HD12	3:Q:183:ALA:HB2	1.96	0.46
3:Q:72:PRO:O	3:Q:76:LEU:HB2	2.16	0.46
1:B:112:LEU:HD11	1:B:120:ARG:NH1	2.30	0.46
2:M:169:SER:OG	2:M:169:SER:O	2.30	0.46
3:Q:45:LEU:HB3	3:Q:237:ILE:HD13	1.97	0.46
2:M:153:TYR:OH	2:M:179:GLY:O	2.25	0.46
1:a:3:PRO:HG2	4:a:307:HOH:O	2.15	0.46
1:b:257:LEU:CD2	1:b:273:GLN:HE22	2.28	0.46
2:m:5:GLU:OE1	2:m:5:GLU:CA	2.63	0.46
2:m:62:SER:C	2:m:64:THR:N	2.73	0.46
1:B:103:VAL:HG13	1:B:153:GLY:HA2	1.96	0.46
2:M:177:LYS:HE2	3:Q:87:ILE:HG13	1.91	0.46
2:m:32:ARG:CZ	3:q:138:PRO:HG2	2.45	0.46
1:a:230:ASP:OD2	1:a:233:THR:OG1	2.27	0.46
2:M:85:MET:O	2:M:86:ALA:C	2.51	0.46
2:M:169:SER:CB	3:Q:87:ILE:O	2.64	0.46
3:Q:232:THR:C	3:Q:235:ALA:H	2.24	0.46
1:b:268:ASP:HA	1:b:271:ALA:HB3	1.96	0.46
2:m:166:ASP:HB2	2:m:177:LYS:CE	2.45	0.46
3:Q:55:PHE:C	4:Q:308:HOH:O	2.57	0.46
2:m:59:LYS:O	2:m:59:LYS:CD	2.49	0.46
2:M:43:MET:HE3	3:Q:201:GLU:HB2	1.98	0.45
1:a:251:ALA:O	1:a:257:LEU:N	2.45	0.45
1:b:19:LYS:HB3	1:b:19:LYS:NZ	2.30	0.45
1:B:109:ASN:OD1	4:B:307:HOH:O	2.21	0.45
1:a:243:LEU:O	1:a:247:LEU:HG	2.16	0.45
2:m:60:ILE:HD12	2:m:60:ILE:HA	1.37	0.45
2:m:63:VAL:HG12	2:m:64:THR:HG23	1.97	0.45
3:q:56:LEU:HD12	4:q:314:HOH:O	2.01	0.45
2:M:95:PHE:O	2:M:99:LEU:HB2	2.17	0.45
3:q:58:ALA:HB1	4:q:315:HOH:O	2.15	0.45
1:A:14:PHE:C	1:A:16:GLY:H	2.24	0.45
2:M:116:ALA:O	2:M:120:PRO:HG2	2.16	0.45
1:b:277:TRP:CA	1:b:278:THR:CB	2.74	0.45
1:a:88:GLN:HG3	1:a:166:GLU:HB2	1.99	0.45
1:A:270:LEU:O	1:A:274:MET:HG3	2.16	0.45
2:M:166:ASP:OD1	2:M:166:ASP:C	2.60	0.45
3:Q:76:LEU:CD2	3:Q:76:LEU:C	2.89	0.45
1:b:99:VAL:O	1:b:103:VAL:HG23	2.17	0.45
1:A:64:LEU:C	1:A:66:GLY:H	2.25	0.45
2:M:55:LEU:C	2:M:57:ALA:H	2.24	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:243:LEU:O	1:a:243:LEU:HG	2.11	0.45
1:b:110:LEU:HD23	1:b:110:LEU:HA	1.80	0.45
1:b:110:LEU:HD11	1:b:157:MET:HB3	1.99	0.45
3:Q:133:ARG:HE	3:Q:134:ARG:HG3	1.81	0.45
3:Q:115:CYS:O	3:Q:118:PHE:HB3	2.17	0.44
1:a:161:VAL:HG22	1:a:192:THR:HB	1.99	0.44
1:a:263:LEU:CD2	1:a:263:LEU:O	2.58	0.44
1:A:112:LEU:N	1:A:112:LEU:HD23	2.32	0.44
1:B:96:ALA:CB	1:B:138:THR:OG1	2.65	0.44
3:Q:19:PRO:CB	3:Q:222:ALA:HB2	2.47	0.44
1:a:87:LEU:HD11	3:q:165:ALA:HB2	1.99	0.44
2:m:10:VAL:HB	3:q:35:VAL:HG12	1.98	0.44
3:q:190:LEU:HB3	3:q:191:PRO:HD3	1.97	0.44
1:A:168:THR:HG21	1:A:176:THR:HG23	1.99	0.44
1:B:14:PHE:CE2	1:B:20:ALA:HB2	2.52	0.44
2:M:116:ALA:O	2:M:117:ILE:C	2.58	0.44
3:Q:19:PRO:HB2	3:Q:222:ALA:HB2	2.00	0.44
1:a:24:LEU:HD11	1:a:213:PHE:HZ	1.81	0.44
1:b:72:SER:HB3	1:b:75:ASP:OD2	2.17	0.44
2:m:2:HIS:CD2	2:m:115:MET:CE	2.99	0.44
1:A:118:ARG:CZ	1:A:134:ARG:HH21	2.28	0.44
1:a:214:ARG:HH11	1:a:219:LEU:HD11	1.83	0.44
1:a:251:ALA:CB	1:a:256:LEU:HB2	2.45	0.44
2:m:43:MET:HE1	3:q:210:GLN:NE2	2.32	0.44
2:m:146:PHE:O	2:m:150:LEU:HB2	2.17	0.44
3:q:19:PRO:CB	3:q:222:ALA:HB2	2.47	0.44
1:A:36:ILE:HG12	1:A:196:SER:CA	2.43	0.44
1:A:279:ARG:HG2	1:B:278:THR:HG22	2.00	0.44
3:Q:15:TRP:CD1	3:Q:58:ALA:HA	2.52	0.44
3:q:73:LEU:HA	4:q:306:HOH:O	2.17	0.44
1:A:64:LEU:HD21	1:A:82:ARG:HD3	1.99	0.44
1:B:128:LEU:HD22	1:B:148:ARG:O	2.17	0.44
1:a:247:LEU:N	1:a:247:LEU:HD23	2.32	0.44
1:a:266:THR:O	1:a:267:ARG:C	2.57	0.44
2:M:200:VAL:HG12	2:M:204:LEU:HD22	1.98	0.44
1:a:265:LYS:HG3	1:a:266:THR:CG2	2.43	0.44
3:q:58:ALA:CB	4:q:305:HOH:O	2.32	0.44
1:A:14:PHE:C	1:A:16:GLY:N	2.75	0.44
1:B:44:LYS:HE2	1:B:44:LYS:HB2	1.64	0.44
1:B:100:PHE:CD2	3:Q:218:THR:HG23	2.53	0.44
2:M:177:LYS:HE3	3:Q:87:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:233:LEU:HD23	3:Q:233:LEU:O	2.18	0.44
1:a:36:ILE:HB	1:a:196:SER:HA	2.00	0.44
1:a:39:PRO:HD3	1:a:237:VAL:HB	2.00	0.44
2:M:7:TYR:OH	3:Q:79:GLY:HA3	2.17	0.43
3:Q:38:PRO:HA	3:Q:39:PRO:HD3	1.90	0.43
2:m:105:LEU:HG	3:q:116:LEU:HD13	2.00	0.43
2:M:4:MET:HE1	3:Q:72:PRO:O	2.17	0.43
3:q:150:ARG:O	3:q:150:ARG:HG2	2.16	0.43
1:A:125:LEU:HB3	1:A:131:SER:HA	2.00	0.43
1:B:261:ALA:HB1	1:B:262:PRO:CG	2.48	0.43
2:M:18:LEU:O	2:M:22:PRO:HD3	2.18	0.43
1:a:197:THR:OG1	1:a:199:ASP:N	2.51	0.43
1:b:72:SER:N	1:b:75:ASP:HB2	2.33	0.43
2:m:42:ARG:NE	3:q:211:GLY:O	2.52	0.43
3:q:137:VAL:HA	3:q:138:PRO:HD3	1.75	0.43
3:Q:20:LEU:HD13	3:Q:127:ASP:HB3	2.01	0.43
1:b:274:MET:HE2	1:b:274:MET:HB3	1.77	0.43
1:b:277:TRP:N	1:b:277:TRP:CD1	2.83	0.43
3:q:19:PRO:HG2	3:q:222:ALA:HA	2.00	0.43
3:q:235:ALA:HA	3:q:238:LEU:HB3	2.00	0.43
3:Q:150:ARG:O	3:Q:150:ARG:HG2	2.16	0.43
3:Q:70:VAL:C	3:Q:72:PRO:HD2	2.43	0.43
3:Q:137:VAL:HA	3:Q:138:PRO:HD3	1.94	0.43
1:A:279:ARG:HG2	1:B:278:THR:HG21	1.99	0.43
2:M:5:GLU:HG3	3:Q:112:ALA:HB1	2.00	0.43
1:a:257:LEU:HD12	1:a:257:LEU:HA	1.65	0.43
1:b:8:GLU:HG3	1:b:61:ARG:HE	1.83	0.43
1:b:21:LEU:HD11	1:b:47:LEU:HA	2.00	0.43
2:m:1:MET:CG	2:m:186:GLN:NE2	2.81	0.43
1:B:259:PRO:O	1:B:260:GLU:HB3	2.19	0.43
3:Q:235:ALA:HA	3:Q:238:LEU:CB	2.48	0.43
1:b:12:TYR:HE2	1:b:14:PHE:CE1	2.37	0.43
1:b:36:ILE:HD13	1:b:36:ILE:HG21	1.76	0.43
3:q:76:LEU:O	3:q:80:ALA:N	2.48	0.43
2:M:205:ALA:O	2:M:206:GLY:C	2.60	0.43
3:Q:73:LEU:HD12	3:Q:74:GLY:N	2.33	0.43
2:m:164:TYR:CZ	3:q:105:LEU:HD12	2.53	0.43
3:Q:38:PRO:HG2	3:Q:241:GLY:O	2.18	0.43
1:a:241:PRO:C	1:a:242:PRO:O	2.55	0.43
2:m:147:LEU:HD23	2:m:147:LEU:HA	1.86	0.43
1:a:45:SER:OG	1:a:165:ASP:OD2	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:2:HIS:ND1	2:m:102:HIS:HD2	2.09	0.42
3:q:226:VAL:O	3:q:229:LEU:HB3	2.19	0.42
3:Q:2:SER:O	3:Q:5:SER:OG	2.32	0.42
3:Q:226:VAL:HA	3:Q:229:LEU:HB3	2.01	0.42
1:B:74:LYS:HE2	1:B:74:LYS:HB3	1.72	0.42
1:B:145:GLN:O	1:B:149:VAL:HG23	2.19	0.42
3:Q:18:ARG:HA	3:Q:18:ARG:HD3	1.37	0.42
3:Q:223:SER:C	3:Q:225:ARG:N	2.77	0.42
1:a:107:PRO:O	1:a:110:LEU:HB2	2.18	0.42
3:q:74:GLY:C	4:q:306:HOH:O	2.61	0.42
1:A:245:ILE:HD11	1:A:265:LYS:HG3	2.02	0.42
1:B:121:VAL:O	1:B:125:LEU:HG	2.20	0.42
1:a:100:PHE:CD1	1:a:121:VAL:HG11	2.54	0.42
3:Q:74:GLY:O	3:Q:75:PHE:C	2.61	0.42
1:a:12:TYR:HA	1:a:58:GLN:HG2	2.01	0.42
1:b:253:ASP:OD1	1:b:253:ASP:N	2.52	0.42
2:m:167:PRO:CB	3:q:86:GLN:HE22	2.25	0.42
1:B:132:ASP:OD1	1:B:132:ASP:N	2.52	0.42
3:Q:234:GLN:O	3:Q:238:LEU:HB2	2.19	0.42
1:a:14:PHE:C	1:a:16:GLY:N	2.77	0.42
1:b:148:ARG:NE	1:b:178:GLN:HE22	2.18	0.42
2:m:53:PHE:HE2	3:q:3:ILE:HD12	1.85	0.42
2:m:55:LEU:C	2:m:57:ALA:N	2.78	0.42
3:q:1:MET:HE2	3:q:1:MET:HB2	1.95	0.42
1:A:35:ALA:HB2	1:A:195:PHE:CZ	2.55	0.42
1:A:256:LEU:HD23	1:B:278:THR:O	2.12	0.42
1:B:274:MET:HE2	1:B:274:MET:HB3	1.86	0.42
3:q:56:LEU:CD1	4:q:318:HOH:O	2.47	0.42
1:B:225:GLU:CG	1:B:226:ALA:N	2.72	0.42
2:m:31:ILE:HA	2:m:34:ILE:HD12	2.02	0.42
3:q:15:TRP:HB2	3:q:58:ALA:HB2	2.02	0.42
1:B:23:ASP:C	1:B:217:ARG:NH1	2.75	0.42
2:M:28:ALA:N	2:M:87:VAL:HG21	2.35	0.42
2:M:166:ASP:CB	2:M:177:LYS:NZ	2.83	0.42
2:M:207:LYS:HZ3	3:Q:191:PRO:CB	2.32	0.42
1:b:147:ARG:NE	1:b:167:PRO:O	2.53	0.42
3:q:219:ARG:HA	3:q:220:PRO:HD3	1.84	0.42
2:M:204:LEU:HD13	3:Q:187:ALA:HB1	2.02	0.42
3:Q:227:LEU:O	3:Q:231:LEU:HB2	2.20	0.42
1:a:261:ALA:HA	1:a:262:PRO:HD3	1.70	0.42
2:m:25:VAL:O	2:m:29:LEU:HD13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:SER:C	1:A:114:GLU:HG2	2.45	0.41
2:M:106:THR:HG21	3:Q:35:VAL:HG21	2.02	0.41
1:b:209:ARG:NH1	1:b:221:GLU:OE1	2.48	0.41
1:A:76:LEU:HD23	1:A:76:LEU:HA	1.76	0.41
1:a:243:LEU:CD1	1:b:267:ARG:HG3	2.50	0.41
1:a:266:THR:O	1:a:270:LEU:HB2	2.20	0.41
1:b:4:ILE:HG22	1:b:28:VAL:O	2.20	0.41
1:b:47:LEU:HD22	1:b:213:PHE:CZ	2.53	0.41
1:b:278:THR:O	1:b:279:ARG:HB2	2.20	0.41
3:q:122:THR:OG1	3:q:123:THR:OG1	2.30	0.41
1:A:120:ARG:HD2	1:A:156:ALA:O	2.20	0.41
1:B:262:PRO:O	1:B:264:PRO:HD3	2.20	0.41
2:M:128:LYS:HE3	2:M:128:LYS:HB2	1.84	0.41
1:b:256:LEU:HB3	1:b:277:TRP:CE2	2.55	0.41
2:m:97:ALA:HB2	2:m:104:GLY:H	1.85	0.41
2:m:170:GLY:CA	2:m:171:PHE:C	2.92	0.41
1:B:122:GLU:OE1	1:B:134:ARG:NH2	2.28	0.41
2:M:170:GLY:O	2:M:173:GLY:N	2.53	0.41
3:Q:211:GLY:O	3:Q:212:GLU:HB2	2.20	0.41
3:q:68:VAL:CA	4:q:301:HOH:O	2.68	0.41
1:A:100:PHE:CD1	1:A:100:PHE:C	2.99	0.41
2:M:31:ILE:O	2:M:35:VAL:HG23	2.20	0.41
2:M:43:MET:HB3	3:Q:197:ALA:HB1	2.02	0.41
2:m:28:ALA:O	2:m:32:ARG:HG3	2.20	0.41
2:m:170:GLY:CA	2:m:173:GLY:H	2.14	0.41
1:A:29:PRO:HG3	1:A:209:ARG:HD2	2.01	0.41
1:B:110:LEU:HD23	1:B:110:LEU:HA	1.84	0.41
1:B:117:ALA:O	1:B:121:VAL:HG23	2.20	0.41
1:B:166:GLU:N	1:B:167:PRO:CD	2.82	0.41
2:M:30:LYS:HG2	2:M:34:ILE:HD11	2.02	0.41
1:a:117:ALA:O	1:a:121:VAL:HG23	2.21	0.41
1:A:173:LEU:HD21	1:B:240:ARG:HG3	2.02	0.41
2:M:73:THR:HG23	2:M:120:PRO:HD3	2.03	0.41
3:Q:70:VAL:O	3:Q:70:VAL:HG12	2.21	0.41
1:a:98:THR:OG1	1:a:101:GLU:HG3	2.21	0.41
1:a:279:ARG:HG2	1:b:278:THR:HG1	1.81	0.41
1:b:54:THR:HG21	3:q:202:THR:HG23	2.02	0.41
3:Q:52:ALA:C	3:Q:56:LEU:HB3	2.46	0.41
3:Q:210:GLN:HB2	3:Q:211:GLY:H	1.29	0.41
1:B:209:ARG:NH2	1:B:222:GLY:HA2	2.36	0.41
3:Q:72:PRO:O	3:Q:73:LEU:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:75:PHE:CD2	3:Q:75:PHE:C	2.99	0.41
1:b:122:GLU:OE1	1:b:134:ARG:NH2	2.40	0.41
1:b:262:PRO:HB2	1:b:263:LEU:H	1.74	0.41
2:m:153:TYR:HE1	2:m:182:PHE:CB	2.34	0.41
2:m:153:TYR:CD1	2:m:186:GLN:HG3	2.56	0.41
3:q:155:LEU:HD23	3:q:155:LEU:HA	1.91	0.41
1:A:39:PRO:HD3	1:A:237:VAL:HB	2.03	0.41
1:A:48:LEU:HD23	1:A:48:LEU:HA	1.86	0.41
1:A:49:LEU:HD22	1:A:54:THR:HG21	2.03	0.41
1:A:244:VAL:HG11	1:A:266:THR:N	2.35	0.41
1:A:278:THR:O	1:A:278:THR:OG1	2.29	0.41
1:a:76:LEU:HD23	1:a:76:LEU:HA	1.80	0.41
1:a:195:PHE:CZ	1:a:207:ALA:HB2	2.56	0.41
1:a:243:LEU:CD2	1:b:247:LEU:CD1	2.97	0.41
1:b:251:ALA:O	1:b:254:HIS:N	2.43	0.41
3:q:210:GLN:C	3:q:210:GLN:CD	2.88	0.41
2:M:60:ILE:HA	2:M:60:ILE:HD13	1.63	0.40
2:M:71:THR:H	2:M:193:GLU:CD	2.28	0.40
2:M:147:LEU:HD23	2:M:147:LEU:HA	1.86	0.40
3:Q:51:LEU:O	3:Q:55:PHE:HD1	2.03	0.40
3:q:89:PRO:CD	3:q:90:GLU:H	2.34	0.40
1:A:37:LEU:HD11	1:A:200:VAL:HG12	2.01	0.40
1:A:261:ALA:HA	1:A:262:PRO:HD3	1.96	0.40
1:B:263:LEU:HD23	1:B:263:LEU:HA	1.85	0.40
2:M:112:ALA:O	2:M:116:ALA:HB3	2.21	0.40
2:M:115:MET:H	2:M:115:MET:HG2	1.58	0.40
1:a:145:GLN:O	1:a:149:VAL:HG23	2.21	0.40
1:a:152:ALA:HA	1:a:155:VAL:HG22	2.03	0.40
1:b:97:THR:C	1:b:98:THR:HG22	2.47	0.40
3:q:52:ALA:O	3:q:56:LEU:HB3	2.21	0.40
1:a:29:PRO:HG3	1:a:209:ARG:HD2	2.02	0.40
1:b:261:ALA:HB1	1:b:262:PRO:CA	2.37	0.40
1:b:271:ALA:O	1:b:274:MET:HB2	2.22	0.40
1:a:241:PRO:HB2	1:a:246:ASP:HB2	2.03	0.40
2:m:113:PHE:O	2:m:114:SER:C	2.58	0.40
3:q:151:PHE:HD2	3:q:151:PHE:HA	1.75	0.40
1:A:26:LEU:HD21	1:A:34:LEU:HD21	2.04	0.40
1:a:241:PRO:O	1:a:242:PRO:C	2.55	0.40
1:b:48:LEU:HA	1:b:48:LEU:HD23	1.88	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Q:232:THR:CG2	3:q:232:THR:OG1[4_568]	1.28	0.92
3:Q:232:THR:CG2	3:q:232:THR:CB[4_568]	2.14	0.06

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	278/280 (99%)	260 (94%)	14 (5%)	4 (1%)	9	26
1	B	278/280 (99%)	267 (96%)	9 (3%)	2 (1%)	18	44
1	a	277/280 (99%)	259 (94%)	14 (5%)	4 (1%)	9	26
1	b	278/280 (99%)	264 (95%)	9 (3%)	5 (2%)	6	21
2	M	205/222 (92%)	191 (93%)	12 (6%)	2 (1%)	12	35
2	m	203/222 (91%)	188 (93%)	11 (5%)	4 (2%)	6	18
3	Q	241/244 (99%)	223 (92%)	14 (6%)	4 (2%)	7	22
3	q	240/244 (98%)	219 (91%)	16 (7%)	5 (2%)	5	17
All	All	2000/2052 (98%)	1871 (94%)	99 (5%)	30 (2%)	8	25

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	263	LEU
1	B	262	PRO
2	M	72	GLY
1	a	262	PRO
1	a	263	LEU
1	a	264	PRO
1	b	278	THR
2	m	9	PRO
2	m	72	GLY
2	m	103	GLY
3	q	73	LEU

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Mol	Chain	Res	Type
3	q	89	PRO
1	A	17	GLY
1	A	114	GLU
1	A	262	PRO
1	B	97	THR
3	Q	210	GLN
1	b	279	ARG
3	q	92	ILE
3	Q	212	GLU
1	a	251	ALA
1	b	260	GLU
2	m	64	THR
3	q	208	ASN
3	Q	96	PRO
1	b	97	THR
3	Q	89	PRO
1	b	16	GLY
2	M	103	GLY
3	q	96	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	208/209 (100%)	195 (94%)	13 (6%)	16	41
1	B	209/209 (100%)	203 (97%)	6 (3%)	37	70
1	a	208/209 (100%)	188 (90%)	20 (10%)	8	23
1	b	209/209 (100%)	191 (91%)	18 (9%)	10	28
2	M	144/155 (93%)	125 (87%)	19 (13%)	4	12
2	m	143/155 (92%)	127 (89%)	16 (11%)	6	17
3	Q	179/180 (99%)	161 (90%)	18 (10%)	7	21
3	q	178/180 (99%)	158 (89%)	20 (11%)	6	17
All	All	1478/1506 (98%)	1348 (91%)	130 (9%)	9	27

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	59	SER
1	A	81	ARG
1	A	97	THR
1	A	112	LEU
1	A	114	GLU
1	A	116	GLU
1	A	122	GLU
1	A	197	THR
1	A	240	ARG
1	A	260	GLU
1	A	263	LEU
1	A	279	ARG
1	B	58	GLN
1	B	74	LYS
1	B	97	THR
1	B	101	GLU
1	B	257	LEU
1	B	262	PRO
2	M	10	VAL
2	M	29	LEU
2	M	34	ILE
2	M	59	LYS
2	M	60	ILE
2	M	63	VAL
2	M	64	THR
2	M	68	SER
2	M	83	SER
2	M	84	VAL
2	M	115	MET
2	M	118	VAL
2	M	120	PRO
2	M	166	ASP
2	M	169	SER
2	M	185	THR
2	M	193	GLU
2	M	204	LEU
2	M	207	LYS
3	Q	5	SER
3	Q	17	SER
3	Q	18	ARG
3	Q	71	LEU

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Mol	Chain	Res	Type
3	Q	73	LEU
3	Q	75	PHE
3	Q	76	LEU
3	Q	90	GLU
3	Q	92	ILE
3	Q	142	ILE
3	Q	157	GLU
3	Q	164	THR
3	Q	166	GLN
3	Q	210	GLN
3	Q	213	MET
3	Q	215	VAL
3	Q	217	SER
3	Q	225	ARG
1	a	1	MET
1	a	2	THR
1	a	59	SER
1	a	74	LYS
1	a	155	VAL
1	a	182	LEU
1	a	195	PHE
1	a	197	THR
1	a	214	ARG
1	a	236	LYS
1	a	240	ARG
1	a	243	LEU
1	a	249	LEU
1	a	250	LEU
1	a	257	LEU
1	a	259	PRO
1	a	263	LEU
1	a	265	LYS
1	a	267	ARG
1	a	270	LEU
1	b	18	VAL
1	b	19	LYS
1	b	58	GLN
1	b	71	HIS
1	b	72	SER
1	b	74	LYS
1	b	97	THR
1	b	98	THR

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Mol	Chain	Res	Type
1	b	113	SER
1	b	166	GLU
1	b	225	GLU
1	b	250	LEU
1	b	252	ARG
1	b	253	ASP
1	b	265	LYS
1	b	267	ARG
1	b	279	ARG
1	b	280	ARG
2	m	8	LEU
2	m	10	VAL
2	m	34	ILE
2	m	59	LYS
2	m	60	ILE
2	m	67	CYS
2	m	68	SER
2	m	84	VAL
2	m	85	MET
2	m	115	MET
2	m	117	ILE
2	m	128	LYS
2	m	132	LYS
2	m	171	PHE
2	m	172	LEU
2	m	193	GLU
3	q	1	MET
3	q	2	SER
3	q	17	SER
3	q	63	ARG
3	q	85	ILE
3	q	86	GLN
3	q	90	GLU
3	q	92	ILE
3	q	122	THR
3	q	123	THR
3	q	175	ARG
3	q	182	THR
3	q	209	TRP
3	q	212	GLU
3	q	215	VAL
3	q	223	SER

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Mol	Chain	Res	Type
3	q	227	LEU
3	q	231	LEU
3	q	232	THR
3	q	233	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	58	GLN
1	B	93	GLN
2	M	102	HIS
2	M	186	GLN
3	Q	234	GLN
1	b	178	GLN
1	b	273	GLN
2	m	12	HIS
2	m	102	HIS
2	m	186	GLN
3	q	86	GLN
3	q	172	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	280/280 (100%)	0.18	8 (2%) 53 46	25, 43, 74, 112	0
1	B	280/280 (100%)	-0.06	5 (1%) 67 60	21, 38, 70, 106	0
1	a	279/280 (99%)	0.50	24 (8%) 16 13	29, 53, 100, 130	0
1	b	280/280 (100%)	0.41	19 (6%) 23 18	27, 48, 96, 170	0
2	M	207/222 (93%)	0.03	7 (3%) 48 41	23, 37, 66, 121	0
2	m	205/222 (92%)	0.10	8 (3%) 43 36	20, 39, 71, 131	0
3	Q	243/244 (99%)	0.35	16 (6%) 24 19	20, 44, 80, 115	0
3	q	242/244 (99%)	0.28	16 (6%) 24 19	23, 45, 80, 116	0
All	All	2016/2052 (98%)	0.23	103 (5%) 33 27	20, 44, 89, 170	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	207	LYS	5.3
1	A	280	ARG	4.6
1	a	266	THR	4.5
1	b	261	ALA	4.3
1	b	262	PRO	4.2
2	m	1	MET	4.2
1	b	280	ARG	4.1
1	a	264	PRO	4.1
3	q	211	GLY	4.0
1	b	259	PRO	3.9
2	m	67	CYS	3.7
3	Q	243	LEU	3.7
1	a	254	HIS	3.6
1	a	270	LEU	3.6
3	q	239	ALA	3.5
1	a	15	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	114	GLU	3.4
3	q	88	GLY	3.4
3	q	241	GLY	3.4
1	a	279	ARG	3.4
3	Q	56	LEU	3.4
1	a	258	ALA	3.3
2	M	206	GLY	3.3
1	a	246	ASP	3.3
2	m	66	SER	3.3
3	Q	241	GLY	3.3
1	a	274	MET	3.2
1	b	255	GLY	3.2
3	Q	227	LEU	3.1
3	Q	88	GLY	3.1
1	a	262	PRO	3.1
1	a	153	GLY	3.1
1	B	71	HIS	3.0
1	B	280	ARG	3.0
1	B	261	ALA	3.0
2	M	66	SER	2.8
1	a	250	LEU	2.8
1	b	263	LEU	2.8
1	A	18	VAL	2.8
1	a	272	ALA	2.8
1	b	260	GLU	2.8
2	m	171	PHE	2.7
3	q	231	LEU	2.7
1	A	139	HIS	2.6
1	a	248	ALA	2.6
3	q	227	LEU	2.6
2	m	32	ARG	2.6
3	Q	222	ALA	2.6
2	M	65	GLY	2.6
2	m	65	GLY	2.6
1	b	264	PRO	2.6
3	q	89	PRO	2.6
3	Q	232	THR	2.5
1	b	251	ALA	2.5
1	a	2	THR	2.5
3	Q	134	ARG	2.5
1	b	248	ALA	2.5
3	Q	1	MET	2.5

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Mol	Chain	Res	Type	RSRZ
3	q	97	ASP	2.5
1	A	14	PHE	2.4
1	A	278	THR	2.4
1	A	35	ALA	2.4
3	Q	224	ALA	2.4
3	q	92	ILE	2.4
3	q	235	ALA	2.4
1	a	245	ILE	2.3
3	Q	87	ILE	2.3
1	b	75	ASP	2.3
1	a	247	LEU	2.3
2	M	62	SER	2.3
3	Q	225	ARG	2.3
1	b	17	GLY	2.3
3	q	238	LEU	2.3
1	b	258	ALA	2.3
1	b	71	HIS	2.3
1	a	256	LEU	2.3
3	Q	231	LEU	2.2
3	q	233	LEU	2.2
3	q	133	ARG	2.2
1	b	277	TRP	2.2
1	a	261	ALA	2.2
1	b	249	LEU	2.2
2	M	1	MET	2.2
2	m	63	VAL	2.2
1	a	251	ALA	2.1
1	A	15	PRO	2.1
1	b	276	GLY	2.1
1	B	14	PHE	2.1
3	q	224	ALA	2.1
3	Q	209	TRP	2.1
3	q	209	TRP	2.1
3	Q	240	ALA	2.1
2	m	64	THR	2.1
2	M	63	VAL	2.1
1	a	14	PHE	2.1
1	a	277	TRP	2.1
1	B	127	ALA	2.0
3	Q	173	ALA	2.0
1	a	1	MET	2.0
1	b	58	GLN	2.0

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Mol	Chain	Res	Type	RSRZ
1	b	254	HIS	2.0
3	q	236	ALA	2.0
1	a	278	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.